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EXPLICIT PATHWISE EXPANSION FOR MULTIVARIATE DIFFUSIONS WITH APPLICATIONS

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Abstract

In this paper, we introduce a unified framework based on the pathwise expansion method to derive explicit recursive formulas for cumulative distribution functions, option prices, and transition densities in multivariate diffusion models. A key innovation of our approach is the introduction of the quasi-Lamperti transform, which normalizes the diffusion matrix at the initial time. This transformation facilitates expansions using uncorrelated Brownian motions, effectively reducing multivariate problems to one-dimensional computations. Consequently, both the analysis and the computation are significantly simplified. We also present two novel applications of the pathwise expansion method. Specifically, we employ the proposed framework to compute the value-at-risk for stock portfolios and to evaluate complex derivatives, such as forward-starting options. Our method has the flexibility to accommodate models with diverse features, including stochastic risk premiums, stochastic volatility, and nonaffine structures. Numerical experiments demonstrate the accuracy and computational efficiency of our approach. In addition, as a theoretical contribution, we establish an equivalence between the pathwise expansion method and the Hermite polynomial-based expansion method in the literature.

Keywords: Pathwise expansion; quasi-Lamperti transform; Hermite expansion; portfolio value-at-risk; forward-starting option

2020 Mathematics Subject Classification: Primary 60H07; 60H35
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1. Introduction

Multivariate diffusions, governed by stochastic differential equations (SDEs), are widely used in financial economics to model the evolution of economic variables such as prices, stochastic volatilities, interest rates, and other state variables. Transition densities, cumulative distribution functions (CDFs), and option prices play a central role in asset pricing and risk management. However, explicit formulas for these quantities are typically unavailable for most

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multivariate diffusions, particularly for processes with complex features, such as stochastic risk premiums, multiple stochastic volatility factors, and nonaffine structures.

These quantities can all be expressed as conditional expectations of certain functionals on the underlying diffusion processes. In the traditional literature (e.g. [26, 35]), the pathwise expansion method was proposed for obtaining closed-form approximations of these quantities. In this kind of approach, the Itô functional is first expanded along with a small parameter, and then the conditional expectation of the expansion coefficients is computed. Deriving explicit formulas for these conditional expectations is often computationally challenging, as it requires dealing with expectations involving correlated Brownian motions.

In this paper, we present a unified framework based on the pathwise expansion method to derive explicit recursive formulas for CDFs, option prices, and transition densities in multivariate diffusion models. To address the aforementioned challenges traditionally faced by the pathwise expansion method, we introduce the *quasi-Lamperti transform*, which normalizes the diffusion matrix of the process at the initial time. This critical step allows subsequent expansions to be reduced to computations involving only uncorrelated multidimensional Brownian motions. By using explicit expressions in terms of Hermite polynomials for the conditional expectation of the product of iterated Itô integrals, we derive explicit expressions for the conditional expectation of the pathwise Taylor expansion coefficients.

This paper contributes to the literature in three aspects. First, we derive explicit expansion formulas for the conditional expectation of a 'general function' on multivariate diffusions. The flexibility in choosing the function greatly broadens the applicability of the pathwise expansion approach. For example, by specifying the function as an indicator function, a vanilla option payoff function, or a Dirac delta function, our method produces explicit Hermite polynomial-based expansion formulas for the marginal CDF, the European option price, and the transition density of multivariate diffusion models. These results have important applications in financial econometrics and risk management; see Section 5. To the best of our knowledge, the expansion formula for the marginal CDF is new to the literature.

Second, we improve upon the traditional pathwise expansion approach by introducing a quasi-Lamperti transform to simplify computations. The Lamperti transform is widely used in the literature to convert univariate SDEs with state-dependent coefficients into SDEs with constant diffusion coefficients, making the transformed process much more computationally tractable. For instance, Beskos and Roberts [9] and Chen and Huang [12] developed exact simulation schemes for general univariate diffusions after applying the transformation, while Aït-Sahalia [1] constructed closed-form approximations for the transition density of the transformed process. However, it is well known that such a transformation does not generally exist in multivariate settings, unless the underlying process satisfies a commutative condition; see [2]. Unfortunately, most processes of interest in financial applications fail to meet this condition.

Unlike the conventional Lamperti transform, the quasi-Lamperti transform ensures only that the diffusion matrix of the transformed process degenerates to an identity matrix at the initial time (see Subsection 3.2 for a detailed discussion). By leveraging this property in conjunction with a Hermite polynomial-based representation for the conditional expectation of the product of iterated Itô integrals (see Lemma 2), our expansion involves only uncorrelated multidimensional normal densities. This simplification makes explicit expansions computationally feasible. Furthermore, by using Hermite polynomials as the 'general function', our approach (Theorem 2) establishes an equivalence between two existing methodologies in the literature of diffusion process density approximation: the pathwise expansion method of Li [26] and the Hermite expansion method introduced by Yang et al. [36] and Wan and Yang [34].

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Third, we explore new applications of diffusion process expansions. In particular, we use the newly developed expansion formula for the marginal CDF to compute the value-at-risk (VaR) for a portfolio within a multivariate model that incorporates both a stochastic risk premium and a stochastic volatility factor. In addition, we derive closed-form expansion formulas for pricing complex exotic derivatives, such as forward-starting options, under general stochastic volatility models, including various specifications of the volatility process, with an emphasis on nonaffine models. To the best of our knowledge, this work is the first to apply expansion methods to these problems. Numerical experiments further validate the accuracy and computational efficiency of our formulas.

Related literature. Watanabe [35] developed a rigorous framework for the pathwise expansion of conditional expectations of generalized functions on a given diffusion process, with a particular emphasis on convergence analysis using Malliavin calculus. Building on this foundation, Li [26, 27] applied the pathwise expansion method to derive asymptotic expansions for the transition density and European option prices by treating the Dirac delta function and the option payoff function as separate cases. Extending [26, 27], our method offers a more unified framework for handling different types of conditional expectations, enabling the simultaneous derivation of explicit expansions for the transition density function, the CDF, and option prices.

Furthermore, we introduce two methodological innovations over the approach in [26, 27]. First, while Li [26, 27] computed the expansion coefficients recursively using the conditional expectation of the product of iterated Stratonovich integrals, we instead use iterated Itô integrals. This innovation eliminates the need to convert between Stratonovich and Itô formulations. More importantly, we find that the conditional expectation of the product of iterated Itô integrals can be expressed in terms of Hermite polynomials, which, in turn, can be derived through higher-order derivatives of the normal distribution. These key observations significantly simplify subsequent computations involving derivatives and integrals of the normal distribution. In addition, this new approach facilitates comparisons with other expansion methods, as demonstrated in Lemma 2.

Second, Li [26] employed a diagonal matrix transformation that produces a multidimensional correlated Brownian motion as the leading term. In contrast, our quasi-Lamperti transform generates a multidimensional uncorrelated standard Brownian motion as the leading term, whose density function is simply the product of univariate normal density functions. This distinction significantly simplifies the computation of higher-order derivatives and multivariate integrals of the density function, allowing the expansion coefficients to be computed more easily and expressed explicitly.

Various methods for expanding transition densities (likelihood functions) have been explored in the literature. The Kolmogorov method [2] expands transition densities in time and state variables by leveraging Kolmogorov equations to determine the expansion coefficients. Yang et al. [36] proposed a delta expansion based on the Itô–Taylor expansion of the Dirac delta function, while Wan and Yang [34] extended the Hermite expansion of [1] to the multivariate setting, establishing a connection with the delta expansion. Other related works include [4, 5, 8, 13, 14, 17, 29, 39]. In addition, in the context of statistical estimation, Yoshida [37, 38] derived expansions for statistical functionals and established properties of the maximum likelihood estimator.

Similarly, expansion techniques have been widely applied to option pricing. In [11, 24, 25, 27, 32] pathwise expansion methods were employed to approximate option prices. In [6] the option price was inverted to derive a closed-form formula for the implied volatility, and in [7]

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an implied stochastic volatility model based on observed volatility surfaces was proposed. For comprehensive overviews of expansion-based approaches in financial modeling, see [10, 33].

Organization of the paper. The remainder of the paper is organized as follows. Section 2 presents the model setup and the problem formulation. Section 3 uses the pathwise expansion method to transform the conditional expectation of a function into an integral involving its product with the normal distribution. Building on this result, Section 4 derives explicit expansion formulas for the transition density, the CDF, and European option prices by taking the function to be the Dirac delta function, an indicator function, and an option payoff function. Section 5 presents two applications along with numerical experiments that demonstrate the accuracy and efficiency of our formulas. Technical lemmas and proofs, as well as an equivalence result between various density expansions, are provided in the Appendix.

Notation. For ease of exposition, we use the following notational conventions throughout the paper. The positive integer m represents the dimension of the state variable. Let $\mathbb{Z}^m$ be the set of m-dimensional integers, and let $\mathbb{Z}_+^m$ be the subset of $\mathbb{Z}^m$ consisting of elements with nonnegative components. For $h=(h_1, h_2, \dots, h_m) \in \mathbb{Z}_+^m$, define $|h| = \sum_{i=1}^m h_i$ and $h! = h_1! \cdots h_m!$. Let e_i be a special index vector whose ith component is 1 and whose other components are 0. We write $x^h = x_1^{h_1} \cdots x_m^{h_m}$ for any $x=(x_1, \dots, x_m)^\top \in \mathbb{R}^m$, where $^\top$ denotes transposition. Let $\mu \in \mathbb{R}^m$ and $\nu \in \mathbb{R}^{m\times m}$ be a vector and a matrix, respectively. We use either μ_i or $(\mu)_i$ to denote the ith element of the vector μ. Similarly, we denote the (i,j)th element of the matrix ν by ν_{ij} or $(\nu)_{ij}$. Let $\phi(x)$ denote the density of the standard m-dimensional multivariate normal distribution with zero mean and identity variance–covariance matrix, and let $H_h(x)$ denote the corresponding multivariate Hermite polynomial, that is, $H_h(x) = (-1)^{|h|}\phi^{-1}(x)\partial_x^h \phi(x)$, where $\partial_x^h = \partial^{|h|}/(\partial x_1^{h_1} \cdots \partial x_m^{h_m})$. In particular, $H_h(x) = \prod_{i=1}^m H_{h_i}(x_i)$, where $H_{h_i}(x_i)$ is the h_ith-order standard univariate Hermite polynomial.

2. The model and problem

Consider a multivariate time-homogeneous diffusion process

$$\mathrm{d}X(s) = \mu^X(X(s))\,\mathrm{d}t + \sigma^X(X(s))\,\mathrm{d}W(s), \tag{1}$$

where $X(s)$ is an $m\times 1$ vector of state variables in the domain $D_X \subset \mathbb{R}^m$ and $W(s)$ is a m-dimensional standard Brownian motion. The drift vector

$$\mu^X(X(s)) = \big(\mu_1^X(X(s)), \dots, \mu_m^X(X(s))\big) \in \mathbb{R}^m$$

and the volatility (or dispersion) matrix $\sigma^X(X(s)) = (\sigma_{ij}^X(X(s)))_{i,j=1}^m \in \mathbb{R}^{m\times m}$ are explicitly known. For two time points t and t' with $t' > t$, let $p_X(t', x' \mid t, x)$ denote the conditional density of $X(t') = x'$ given $X(t) = x$. The diffusion matrix associated with the process is thus defined as

$$\nu^X(\xi) = \sigma^X(\xi)\big(\sigma^X(\xi)\big)^\top. \tag{2}$$

The primary goal of this paper is to derive a closed-form expansion for the conditional expectation of a given function $g(X(t'))$, conditioned on $X(t) = x$ for $t' > t$. Depending on the application, the function $g(\cdot)$ can take various forms, such as a generalized function (e.g. the Dirac delta function), an indicator function, or a Lipschitz-continuous function. By appropriately choosing $g(\cdot)$, we can derive analytical expressions for the transition densities and

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CDFs of the process X, for instance, as well as for the prices of European options where the underlying asset dynamics are governed by X. To address potential degeneracies in computation when $\Delta = t' - t$ is small, we rescale $X(t')$ by $(X(t') - x)/\sqrt{t' - t}$. Obviously, computing $\mathbb{E}[g(X(t')) \mid X(t) = x]$ is equivalent to computing

$$\mathbb{E}\left[f_X\left(\frac{X(t') - x}{\sqrt{t' - t}} \right) \,\middle|\, X(t) = x \right] \tag{3}$$

if we define $f_X(a) = g(\sqrt{t' - t} \cdot a + x)$. In light of this transformation, we hereafter focus on the expansion of (3) without loss of generality.

Following the technical assumptions in the standard pathwise expansion literature, such as [26, 35], we make the following assumptions.

Assumption 1. *The diffusion matrix $v^X(x)$ is positive definite, i.e. $\zeta^\top v^X(x)\zeta > 0$ for any nonzero vector $\zeta \in \mathbb{R}^m$ and $x \in D_X$.*

Assumption 2. *All the components of $\mu^X(x)$ and $\sigma^X(x)$ are infinitely differentiable with bounded derivatives of all orders.*

Assumptions 1 and 2 are conventionally imposed in the study of SDEs, as discussed in [19]. These assumptions are sufficient, though not necessary, to ensure the existence, uniqueness, and smoothness of the expansion target, such as the transition density function of the process. However, the numerical examples presented in this paper indicate that the proposed method applies to a broad range of commonly used models, extending beyond those that strictly meet these sufficient conditions, for example the SV-1/2 model. This suggests that local relaxations may be feasible for specific models, a direction for future research.

3. Explicit formulas for the conditional expectation via the pathwise expansion method

The expansion process involves the following two main steps.

(i) Pathwise Taylor expansion: Using the chain rule for composite functions and the methods developed in [26, 35], we derive a pathwise Taylor expansion of $f_X\left(\frac{X(t')-x}{\sqrt{t'-t}}\right)$ with respect to $\epsilon = \sqrt{\Delta} = \sqrt{t' - t}$.

(ii) Computation of the conditional expectations of expansion coefficients: We then compute explicit formulas for the conditional expectations of the coefficients in the pathwise Taylor expansion.

The details of each step are elaborated in this section.

3.1. Heuristic idea behind the expansion

Before presenting the technical details of our pathwise expansion method, we discuss the heuristic ideas behind it in this subsection to provide readers with a better understanding of the new contributions of this work relative to the existing literature.

The first step is inspired by Theorem 3.3 of [35]. By introducing a small parameter $\epsilon = \sqrt{\Delta} = \sqrt{t' - t}$, we fix $X(t) = x$ and rescale the process $X(\cdot)$ on the time horizon $[t, +\infty)$ through the transformation $X^\epsilon(s) = X(\epsilon^2 s + t)$ for $s \geq 0$. By (1), the rescaled process satisfies

$$\mathrm{d}X^\epsilon(s) = \epsilon^2 \mu^X(X^\epsilon(s))\,\mathrm{d}s + \epsilon \sigma^X(X^\epsilon(s))\,\mathrm{d}W^\epsilon(s), \quad X^\epsilon(0) = x, \tag{4}$$

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where

$$W^{\epsilon}(s) = \frac{1}{\epsilon} W\big(\epsilon^2 s + t\big).$$

Obviously, $\{W^{\epsilon}(s),\ s \geq 0\}$ is identical to an m-dimensional standard Brownian motion in the probability law. Hereafter we use $W(s)$ to denote $W^{\epsilon}(s)$ for simplicity. Since we are interested in computing expectations of X^{ϵ}, the equivalence between the distributional laws of $W(s)$ and $W^{\epsilon}(s)$ ensures that this abuse of notation will not cause any problems.

Let X_i^{ϵ} represent the ith component of X^{ϵ}, for $1 \leq i \leq m$. Note that the expansion target $X(t') = X^{\epsilon}(1)$. Then, by (4), we have

$$X_i^{\epsilon}(1) - x_i = \epsilon^2 \int_0^1 \mu_i^X(X^{\epsilon}(t_1))\,\mathrm{d}t_1 + \epsilon \sum_{k=1}^{m} \int_0^t \sigma_{i,k}^X(X^{\epsilon}(t_1))\,\mathrm{d}W_k(t_1). \tag{5}$$

Applying Itô's formula to $\sigma_{i,k}^X(X^{\epsilon}(t_1))$ in the term of order ϵ (i.e. the second integral on the right-hand side of (5)) leads to

$$\begin{aligned}
&X_i^{\epsilon}(1) - x_i \\
&= \epsilon^2 \int_0^1 \mu_i^X(X^{\epsilon}(t_1))\,\mathrm{d}t_1 \\
&\quad + \epsilon \sum_{k=1}^{m} \int_0^1 \Bigg[\sigma_{i,k}^X(x) + \epsilon \sum_{l=1}^{m} \int_0^{t_1} \mathcal{L}_x^{X,l} \sigma_{i,k}^X(X^{\epsilon}(t_2))\,\mathrm{d}W_l(t_2) \\
&\qquad\qquad + \epsilon^2 \int_0^{t_1} \mathcal{L}_x^{X,0} \sigma_{i,k}^X(X^{\epsilon}(t_2))\,\mathrm{d}t_2 \Bigg] \mathrm{d}W_k(t_1) \\
&= \epsilon \sum_{k=1}^{m} \sigma_{i,k}^X(x) W_k(1) + \epsilon^2 \int_0^1 \mu_i^X(X^{\epsilon}(t_1))\,\mathrm{d}t_1 \\
&\quad + \epsilon^2 \sum_{k=1}^{m} \sum_{l=1}^{m} \int_0^1 \left(\int_0^{t_1} \mathcal{L}_x^{X,l} \sigma_{i,k}^X(X^{\epsilon}(t_2))\,\mathrm{d}W_l(t_2) \right) \mathrm{d}W_k(t_1) + \mathcal{O}(\epsilon^3),
\end{aligned} \tag{6}$$

where $\mathcal{O}(\epsilon^3)$ represents the terms of order ϵ^3 and higher, and $\{\mathcal{L}_x^{X,l},\ l = 0, 1, \ldots, m\}$ is a set of differential operators associated with the process X such that for a sufficiently smooth function G,

$$\mathcal{L}_x^{X,l} G(x) = \sum_{k=1}^{m} \mu_k^X(x) \partial_x^{e_k} G(x) + \frac{1}{2} \sum_{k,h=1}^{m} \nu_{kj}^X(x) \partial_x^{e_k + e_h} G(x) \quad \text{for } l = 0$$

and

$$\mathcal{L}_x^{X,l} G(x) = \sum_{k=1}^{m} \sigma_{kl}^X(x) \partial_x^{e_k} G(x) \quad \text{for } l = 1, \ldots, m.$$

Our approach builds on the theoretical framework established in [35], which uses Stratonovich integrals in the expression of Itô's formula. However, by working directly with Itô integrals in (6), we circumvent the need for converting Stratonovich integrals into Itô integrals, as outlined in Appendix A.1 of [26]. This refinement significantly simplifies the subsequent computational process, enabling more efficient derivation of explicit formulas.

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We continue applying Itô's formula to the integrands of order ϵ^2 (i.e. the second and third terms on the right-hand side of (6)). After some algebraic operations, we obtain

$$X_i^\epsilon(1) - x_i = \epsilon F_{1,i}^X + \epsilon^2 F_{2,i}^X + \mathcal{O}(\epsilon^3), \tag{7}$$

with

$$F_{1,i}^X = \sum_{k=1}^m \sigma_{i,k}^X(x) W_i(1) = \left(\sigma^X(x) W(1)\right)_i \tag{8}$$

and

$$F_{2,i}^X = \mu_i^X(x) + \sum_{k=1}^m \sum_{l=1}^m \mathcal{L}_x^{X,l} \sigma_{i,k}^X(x) \int_0^1 \int_0^{t_1} \mathrm{d}W_l(t_2)\, \mathrm{d}W_k(t_1). \tag{9}$$

Note that the expansion in (7) works for any component i of the vector X^ϵ. In this way, repeatedly applying Itô's formula to the integrands yields

$$X^\epsilon(1) - x = \epsilon F_1^X + \epsilon^2 F_2^X + \cdots + \epsilon^K F_K^X + \mathcal{O}\left(\epsilon^{K+1}\right) \tag{10}$$

for any order K. We establish the explicit forms for all the coefficients in Lemma 1.

Next, substitute (10) into $f_X(\cdot)$. To help readers more easily grasp the intuition behind our approach, let us temporarily assume that f_X is infinitely differentiable. Then, by applying the chain rule of differentiation for composite functions, we can expand $f_X(\cdot)$ with respect to ϵ:

$$\begin{aligned} f_X\left(\frac{X^\epsilon(1) - x}{\epsilon}\right) &= f_X\left(F_1^X + \epsilon F_2^X + \cdots + \epsilon^{K-1} F_X^K + \mathcal{O}(\epsilon^K)\right) \\ &= f_X(F_1^X) + \sum_{k=1}^{K-1} \epsilon^k \Phi_k^X\left(x; f_X(\cdot)\right) + \mathcal{O}(\epsilon^K), \end{aligned} \tag{11}$$

where the coefficients $\Phi_k^X\left(x; f_X(\cdot)\right)$ $(k = 1, \ldots, K-1)$ are given by the order-k derivatives of $f_X((X^\epsilon(1) - x)/\epsilon)$ with respect to ϵ. Taking the expectation on both sides of (11), we know that

$$\mathbb{E}\left[f_X\left(\frac{X^\epsilon(1) - x}{\epsilon}\right) \,\middle|\, X^\epsilon(0) = x\right] = \mathbb{E}\left[f_X\left(F_1^X\right)\right] + \sum_{k=1}^{K-1} \epsilon^k \mathbb{E}\left[\Phi_k^X\left(x; f_X(\cdot)\right)\right] + \mathcal{O}(\epsilon^K). \tag{12}$$

In light of (12), developing a valid expansion for (3) requires explicitly calculating the conditional expectation of the expansion coefficients $\mathbb{E}[\Phi_k^X(x; f_X(\cdot))]$. This constitutes the second step of our approach, which represents the primary contribution of the paper, as noted in the Introduction. We take the order-0 and order-1 terms in (12), $\mathbb{E}[f_X(F_1^X)]$ and $\mathbb{E}[\Phi_1^X(x; f_X(\cdot))]$, as examples to illustrate how we invoke the quasi-Lamperti transform introduced in Subsection 3.2 to address the difficulties we encounter.

By (8), $F_1^X = \sigma^X(x) W(1)$. It follows a multivariate normal distribution with mean 0 and covariance matrix $\nu^X(x)$. Denote its density at z by $\phi(z; \nu^X(x))$. Thus,

$$\mathbb{E}\left[f_X\left(F_1^X\right)\right] = \int_{\mathbb{R}^m} f_X(z) \phi\left(z; \nu^X(x)\right) \mathrm{d}z. \tag{13}$$

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Meanwhile, noting that

$$\Phi_1^X\big(x; f_X(\cdot)\big) = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left[f_X\Big(\frac{X^\epsilon(1)-x}{\epsilon}\Big)\right]\Big|_{\epsilon=0} = \sum_{i=1}^m \frac{\partial f_X}{\partial z_i}\big(F_1^X\big)\, F_{2,i}^X,$$

we have

$$\begin{aligned}\mathbb{E}\big[\Phi_1^X\big(x; f_X(\cdot)\big)\big] &= \sum_{i=1}^m \mathbb{E}\left[\frac{\partial f_X}{\partial z_i}\big(F_1^X\big)\, F_{2,i}^X\right] \\ &= \sum_{i=1}^m \int_{\mathbb{R}^m} \frac{\partial f_X}{\partial z_i}(z)\, \mathbb{E}\big[F_{2,i}^X \,\big|\, F_1^X = z\big]\, \phi(z; \nu^X(x))\, \mathrm{d}z,\end{aligned}$$

where the second equality is due to the iterated law of conditional expectations and $F_1^X \sim \phi(z; \nu^X(x))$. Substituting the expression for $F_{2,i}^X$ (cf. (9)) into $\mathbb{E}[F_{2,i}^X \mid F_1^X = z]$ leads to

$$\begin{aligned}&\int_{\mathbb{R}^m} \frac{\partial f_X}{\partial z_i}(z)\, \mathbb{E}\big[F_{2,i}^X \,\big|\, F_1^X = z\big]\, \phi(z; \nu^X(x))\, \mathrm{d}z \\ &= \mu_i^X(x) \int_{\mathbb{R}^m} \frac{\partial f_X}{\partial z_i}(z)\phi(z; \nu^X(x))\, \mathrm{d}z + \sum_{k=1}^m \sum_{l=1}^m \mathcal{L}_x^{X,l}\sigma_{i,k}^X(x) \int_{\mathbb{R}^m} \frac{\partial f_X}{\partial z_i}(z)\Pi_{k,l}(z)\phi(z; \nu^X(x))\, \mathrm{d}z,\end{aligned}$$

with

$$\Pi_{k,l}(z) = \mathbb{E}\left[\int_0^1 \int_0^{t_1} \mathrm{d}W_l(t_2)\, \mathrm{d}W_k(t_1) \,\middle|\, \sigma^X(x)W(1) = z\right].$$

Whenever f_X is dominated by a normal density at infinity, we can further use integration by parts to show that

$$\begin{aligned}\int_{\mathbb{R}^m} \frac{\partial f_X}{\partial z_i}(z)\phi\big(z; \nu^X(x)\big)\, \mathrm{d}z &= -\int_{\mathbb{R}^m} f_X(z) \frac{\partial}{\partial z_i}\big(\phi\big(z; \nu^X(x)\big)\big)\, \mathrm{d}z, \\ \int_{\mathbb{R}^m} \frac{\partial f_X}{\partial z_i}(z)\Pi_{k,l}(\hat{z})\phi\big(z; \nu^X(x)\big)\, \mathrm{d}z &= -\int_{\mathbb{R}^m} f_X(z) \frac{\partial}{\partial z_i}\big(\Pi_{k,l}(z)\phi\big(z; \nu^X(x)\big)\big)\, \mathrm{d}z. \end{aligned} \tag{14}$$

Thus, to compute the expansion coefficients, we need to evaluate the multidimensional integrals on the right-hand side of (14). For higher-order terms, this task becomes increasingly challenging as the first-order terms in (14) are replaced by higher-order partial derivatives with respect to z. However, one special case is tractable: when $\sigma^X(x)$ is an identity matrix. In this case, the correlated normal density function $\phi(z; \nu^X(x))$ in (14) simplifies to an uncorrelated standard normal density function $\phi(z)$, which can be expressed as a product of multiple univariate normal density functions. In addition, when $\sigma^X(x)$ is an identity matrix, $\Pi_{k,l}(z)$ also becomes computable as follows:

$$\Pi_{k,l}(z) = \mathbb{E}\left[\int_0^1 \int_0^{t_1} \mathrm{d}W_l(t_2)\, \mathrm{d}W_k(t_1) \,\middle|\, W(1) = z\right] = \begin{cases} \frac{1}{2}\big(z_k^2 - 1\big) & \text{if } l = k, \\ \frac{1}{2} z_l z_k & \text{if } l \neq k. \end{cases}$$

From $\Pi_{k,l}$, we can see the aforementioned advantage of working directly with Itô integrals instead of Stratonovich integrals, because the former admit closed-form representations, as

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shown above. In Lemma 2, we generalize this result about $\Pi_{k,l}(z)$ by representing the conditional expectation of a product of iterated Itô integrals as a linear combination of products of one-dimensional Hermite polynomials. Leveraging these observations, we can derive an explicit form for the expansion of (3) when $\sigma^X(x)$ is an identity matrix.

The introduction of the *quasi-Lamperti transform* in the next subsection allows us to extend this tractability to address computational challenges in the general case. This transform maps the original process X to a new process Y with an identity diffusion matrix at the initial time. Working with the transformed process Y in Subsection 3.3, we derive an explicit expansion formula for the expectation (3); see Theorem 1.

The close relationship between the conditional expectations of iterated Itô integrals and Hermite polynomials once again plays a crucial role in simplifying the calculations. Specifically, we reduce the computation of the expansion coefficients to evaluating the following integral:

$$\int_{\mathbb{R}^m} f(z) \frac{\partial^k}{\partial z_i^k} \left(\prod_{j=1}^{m} H_{h_j}\left(z_j\right) \phi(z_j) \right) \mathrm{d}z, \tag{15}$$

where $f(\cdot)$ is the corresponding function of f_X under the transformed process Y, $H_{h_j}(z_j)$ is the h_jth-order univariate Hermite polynomial, and $\phi(z_j)$ is the univariate standard normal density function. Thanks to the special structure of Hermite polynomials, we can relate its high-order derivatives to a combination of itself and standard normal distribution densities. This key observation helps us avoid the step of evaluating $\partial^k/\partial z_i^k\big(\prod_{j=1}^m H_{h_j}(z_j)\phi(z_j)\big)$, which requires significant computational effort.

Remark 1. It is unnecessary for f_X to be infinitely differentiable in our expansion approach. Specifically, (14) holds when f_X is differentiable in a weak sense. More precisely, if we aim to expand up to K th order, we only require f_X to belong to the Sobolev space $W^{K,1}(\mathbb{R}^m, \mu)$, where μ is the measure induced by the standard uncorrelated normal distribution on $\mathbb{R}^m$. This means that $f_X \in L^1(\mathbb{R}^m, \mu)$ and all weak derivatives of f_X up to order K also belong to $L^1(\mathbb{R}^m, \mu)$.

3.2. Quasi-Lamperti transform $X \to Y$

Now we formally introduce the quasi-Lamperti transform and start the rigorous derivation. For a fixed initial time t and state $X(t) = x$, define a process Y by the linear transformation

$$Y(s) = (\sigma^X(x))^{-1} X(s) = LX(s) \quad \text{for } s \geq t, \tag{16}$$

where $L = (\sigma^X(x))^{-1}$ is the inverse matrix of the volatility matrix σ^X at the initial point x. Then the dynamics of Y satisfy, according to Itô's formula,

$$\mathrm{d}Y(s) = \mu^Y(Y(s))\,\mathrm{d}s + \sigma^Y(Y(s))\,\mathrm{d}W(s), \quad Y(t) = y. \tag{17}$$

Here the initial point for the new process changes to $y = Lx$. Also, the drift vector and volatility matrix of Y are given by $\mu^Y(z) = L\mu^X(L^{-1}z)$ and $\sigma^Y(z) = L\sigma^X(L^{-1}z)$, respectively, for any z. Hence, the diffusion matrix of process Y is

$$\nu^Y(z) = \sigma^Y(z)\sigma^Y(z)^\top = L\sigma^X\left(L^{-1}z\right)\left(\sigma^X\left(L^{-1}z\right)\right)^\top L^\top.$$

In light of the above equality, we can easily see that the initial diffusion matrix of Y must be an identity matrix; that is, upon taking z to be $y = Lx$ in $\nu^Y(z)$,

$$\nu^Y(y) = \sigma^Y(y)\sigma^Y(y)^\top = L\sigma^X(x)\left(\sigma^X(x)\right)^\top L^\top = LL^{-1}(L^\top)^{-1}L^\top = \mathrm{Id}_m.$$

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The transformation defined through (16) is called a *quasi-Lamperti transform*. It is a simple linear transformation. Mimicking $\mathcal{L}^{X,l}$, we can define the corresponding differential operators for Y:

$$\mathcal{L}_\zeta^{Y,0} = \sum_{k=1}^{m} \mu_k^Y(\zeta)\partial_\zeta^{e_k} + \frac{1}{2}\sum_{k,l=1}^{m} \nu_{kj}^Y(\zeta)\partial_\zeta^{e_k+e_l}, \tag{18}$$

$$\mathcal{L}_\zeta^{Y,l} = \sum_{k=1}^{m} \sigma_{kl}^Y(\zeta)\partial_\zeta^{e_k} \quad \text{for } l = 1, \ldots, m. \tag{19}$$

Denote by $p_X(t', x' \mid t, x)$ and $p_Y(t', y' \mid t, y)$ the transition densities for the original process X and the transformed diffusion Y, respectively. By the Jacobian formula for the change of density, we have

$$p_X(t', x' \mid t, x) = \det(L)\, p_Y(t', Lx' \mid t, Lx). \tag{20}$$

Thus, once we have derived a Kth-order density expansion for Y, we can recover a (approximate) density for the original X by using (20).

Remark 2. For univariate diffusions, the volatility σ^X in (1) is a scalar function. The existing literature defines the Lamperti transform in such a way that

$$L(\cdot) = \int_x^{\cdot} \frac{1}{\sigma^X(u)}\,\mathrm{d}u$$

(see e.g. equation (2.1) of [1]). Under it, the transformed process $Y = L(X)$ has a unit volatility independent of its state. This transform is widely used in the literature to make the transformed process more computationally tractable. For instance, in [9, 12] exact simulation schemes were developed for general univariate diffusions after applying the transformation, while in [1] closed-form approximations were constructed for the transition density of the transformed process.

However, a global Lamperti transform does not exist for multivariate diffusion processes, the primary focus of this paper, unless the volatility matrix of the process satisfies a communicative condition as stipulated in Proposition 1 of [2]. The transform introduced in (16) is much weaker in the sense that the diffusion matrix degenerates to an identity matrix only at the initial point $X = x$. It suffices since our goal is to derive a small-time expansion around the initial time. This is because the diffusion matrix of the transformed process will not deviate too much from the identity matrix within a small time horizon.

3.3. The general Kth-order expansion

In this subsection, we apply the procedure outlined in Subsection 3.1 to the transformed process Y to derive the explicit expansion formula up to the Kth order. Similar to (4), we rescale the process by $Y^\epsilon(s) = Y(\epsilon^2 s + t)$ for $s \geq 0$. By (17), we know that this leads to the SDE

$$\mathrm{d}Y^\epsilon(s) = \epsilon^2 \mu^Y(Y^\epsilon(s))\,\mathrm{d}s + \epsilon\sigma^Y(Y^\epsilon(s))\,\mathrm{d}W(s), \qquad Y^\epsilon(0) = y.$$

Note that $Y^\epsilon(1) = Y(t')$ and that the normalization Γ^ϵ satisfies

$$\Gamma^\epsilon = \frac{Y^\epsilon(1) - y}{\epsilon} \to W(1) \quad \text{as } \epsilon \to 0. \tag{21}$$

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This convergence holds because $\sigma^Y(y)$ is an identity matrix. This asymptotic behavior contrasts with that of the original process, where $(X^\epsilon - 1)/\epsilon$ converges to $F_1^X = \sigma^X(x)W(1)$ as $\epsilon \to 0$ (see (7) and (8)), which is a correlated multivariate Brownian motion.

Now we proceed to express the target conditional expectation (3) in terms of Γ^ϵ. First, let $f(z) = f_X(L^{-1}z)$; then we have

$$\mathbb{E}\left[f_X\left(\frac{X(t')-x}{\sqrt{t'-t}}\right)\,\middle|\,X(t)=x\right] = \mathbb{E}\left[f\left(\frac{Y(t')-y}{\sqrt{t'-t}}\right)\,\middle|\,Y(t)=y\right].$$

Using $Y^\epsilon(1) = Y(t')$,

$$\mathbb{E}\left[f\left(\frac{Y(t')-y}{\sqrt{t'-t}}\right)\,\middle|\,Y(t)=y\right] = \mathbb{E}\big[f(\Gamma^\epsilon)\,\big|\,Y^\epsilon(0)=y\big]. \tag{22}$$

The task is now reduced to expanding the conditional expectation in (22).

Remark 3. It is worth noting that the normalization Γ^ϵ here corresponds to the standardization described in equation (3.16) of [26], but there are significant differences between the two approaches. In [26], a diagonal matrix transformation is applied to standardize the original diffusion X, resulting in a multidimensional correlated Brownian motion (see equation (3.17) of [26]). Hence, Li's approach still involves the computation of multidimensional integrals, similar to those in (14). In contrast, our approach employs the quasi-Lamperti transform, where the normalization Γ^ϵ converges to an uncorrelated multidimensional standard Brownian motion W(1). This leads to significantly simpler integrals, as shown in (32). This simplification represents one of the key innovations that distinguish this paper from the method proposed in [26].

3.3.1. *Step 1: Pathwise Taylor expansion of $f(\Gamma^\epsilon(1))$ with respect to ϵ.* Following the approach that led to (10), we establish a pathwise expansion of $Y^\epsilon(1)$ in Lemma 1. The convergence of the expansion is guaranteed by Watanabe theory from Malliavin calculus (see e.g. [26, 27, 35]). It is worth noting that, unlike the original method proposed in [35], our expansion uses iterated Itô integrals. This choice offers significant computational advantages, particularly in the subsequent steps of the procedure.

For ease of exposition, we first define some notation. For any n, consider an index $\mathbf{i} = (i_1, i_2, \ldots, i_n) \in \{0, 1, \ldots, m\}^n$. Define its 'norm' by

$$\|\mathbf{i}\| = \sum_{l=1}^{n} \big(2 \cdot \mathbf{1}_{\{i_l=0\}} + \mathbf{1}_{\{i_l\neq 0\}}\big). \tag{23}$$

For instance, the norms of $\mathbf{i}_1 = (1, 1, \ldots, 1)$ and $\mathbf{i}_2 = (0, 1, \ldots, 1)$ equal n and $n+1$, respectively. In addition, let $\mathcal{M}_k^n$ be the collection of all the n-dimensional indices with norm k, that is,

$$\mathcal{M}_k^n = \{\mathbf{i} = (i_1, i_2, \ldots, i_n) : \|\mathbf{i}\| = k\}.$$

Obviously, $\mathcal{M}_0^n = \emptyset$ for all positive integers n, $\mathcal{M}_1^1 = \{(1), \ldots, (m)\}$ and $\mathcal{M}_1^n = \emptyset$ for $n \geq 2$, and $\mathcal{M}_2^1 = \{(0)\}$. Further, $\mathcal{M}_k^n$ can be constructed in the following recursive way: for $n \geq 2$,

$$\mathcal{M}_{k+1}^n = \big\{\mathbf{i} : i_1 = 0,\ (i_2, \ldots, i_n) \in \mathcal{M}_{k-1}^{n-1}\big\} \cup \left\{\bigcup_{\alpha=1}^{m} \big\{\mathbf{i} : i_1 = \alpha,\ (i_2, \ldots, i_n) \in \mathcal{M}_k^{n-1}\big\}\right\}. \tag{24}$$

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For an index $\mathbf{i} = (i_1, \ldots, i_n) \in \mathcal{M}_k^n$, define

$$C_{\mathbf{i}}^Y(\zeta) = \big(\mathcal{L}_\zeta^{Y,i_n} \circ \cdots \circ \mathcal{L}_\zeta^{Y,i_2}\big)\sigma_{\cdot i_1}^Y(\zeta), \tag{25}$$

where $\sigma_{\cdot 0}^Y = \mu^Y$, $\sigma_{\cdot i_1}^Y = (\sigma_{1i_1}^Y, \ldots, \sigma_{mi_1}^Y)^\top$ and the operator $L_\zeta^{Y,i}$ follows the definition in (18) and (19). Note that in computing $C_{\mathbf{i}}^Y$, we just repeatedly apply differential operations on the elements of the volatility matrix of Y. This step can be easily accomplished by symbolic computation tools such as *Mathematica*.

Let $\mathcal{M}_k = \bigcup_n \mathcal{M}_k^n$. Note that for any given k, there are only finitely many nonempty $\mathcal{M}_k^n$ in the union. We have the following result.

Lemma 1. *Suppose that Assumptions 1 and 2 hold. Then the random variable $Y^\epsilon(1)$ admits the expansion*

$$Y^\epsilon(1) = \sum_{k=0}^K \epsilon^k F_k^Y + \mathcal{O}\big(\epsilon^{K+1}\big).$$

Furthermore, the expansion coefficients satisfy $F_0^Y = y$ and

$$F_k^Y = \sum_{\mathbf{i}\in\mathcal{M}_k} C_{\mathbf{i}}^Y(y) \cdot \mathbb{I}_{\mathbf{i}}(1),$$

where $\mathbb{I}_{\mathbf{i}}(t)$ is an iterated Itô integral defined through

$$\mathbb{I}_{\mathbf{i}}(t) = \int_0^t \int_0^{t_1} \cdots \int_0^{t_{n-1}} \mathrm{d}W_{i_n}(t_n) \cdots \mathrm{d}W_{i_2}(t_2)\, \mathrm{d}W_{i_1}(t_1).$$

Here we take $W_0(t) = t$ by convention.

By replacing X with Y and x with y in (8) and (9), we can see the explicit expressions for the first two terms, F_1^Y and F_2^Y, respectively.

3.3.2. *Step 2: Computation of the conditional expectations of the pathwise Taylor expansion coefficients.* By substituting the pathwise expansion result from Lemma 1 into (21) and combining it with (22), we have

$$\begin{aligned}\mathbb{E}\left[f_X\left(\frac{X(t')-x}{\sqrt{t'-t}}\right)\,\middle|\, X(t)=x\right] &= \mathbb{E}\big[f(\Gamma^\epsilon)\,\big|\, Y(t)=y\big] \\ &= \mathbb{E}\left[f\left(\sum_{j=0}^K F_{j+1}^Y \epsilon^i + \mathcal{O}(\epsilon^{K+1})\right)\,\middle|\, Y(t)=y\right].\end{aligned}$$

The main theorem of this section expands the right-hand side of the above equality with respect to ϵ, yielding

$$\mathbb{E}\left[f_X\left(\frac{X(t')-x}{\sqrt{t'-t}}\right)\,\middle|\, X(t)=x\right] = \Omega_0\big(y; f(\cdot)\big) + \sum_{k=1}^K \Omega_k(y; f(\cdot))\epsilon^k + \mathcal{O}(\epsilon^{K+1}). \tag{26}$$

The most significant contribution of this theorem is that it provides explicit expressions for the expansion coefficients $\Omega_k\big(y; f(\cdot)\big)$.

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We need to introduce some additional notation to make the presentation of the theorem more succinct. First, given any index vector $\mathbf{h} = (h_1, \ldots, h_m) \in \{0, 1, \ldots, m\}^m$, let

$$I(f(\cdot), \mathbf{h}) = \int_{\mathbb{R}^m} f(z) H_{\mathbf{h}}(z) \phi(z)\, \mathrm{d}z. \tag{27}$$

Note that it is independent of the diffusion model. Here, $H_{\mathbf{h}}(\cdot)$ is a multivariate Hermite polynomial indexed by $\mathbf{h}$, as defined at the end of the Introduction. One important observation is that $H_{\mathbf{h}}$ can be decomposed into a product of univariate polynomials; in particular, $H_{\mathbf{h}}(x) = \prod_{i=1}^m H_{h_i}(x_i)$, where $H_{h_i}(x_i)$ is the h_ith-order standard univariate Hermite polynomial.

Second, for any given positive integers l and k, we define

$$\mathcal{S}_k^l = \{\mathbf{j} = (j_1, j_2, \ldots, j_l) : j_\omega \geq 1,\ \omega = 1, \ldots, l;\ j_1 + j_2 + \cdots + j_l = k\} \tag{28}$$

and $\mathcal{S}_k = \bigcup_{l=1}^k \mathcal{S}_k^l$. Obviously,

$$\mathcal{S}_{k+1} = \{\mathbf{j} : j_1 = 1,\ (j_2, \ldots, j_l) \in \mathcal{S}_k\} \cup \{\mathbf{j} : (j_1 - 1, j_2, \ldots, j_l) \in \mathcal{S}_k\}.$$

Third, for any two indices $\mathbf{i}$ and $\mathbf{j}$, where $\mathbf{i}$ and $\mathbf{j}$ are vectors and may have different dimensionalities, define a concatenation operation between these two vectors such that $\mathbf{i} \wedge \mathbf{j}$ is a new index vector obtained by putting $\mathbf{j}$ at the end of $\mathbf{i}$. Repeating this operation, it is easy to get the concatenated index vector $\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l$ for any sequence of indices $\{\mathbf{i}_1, \ldots, \mathbf{i}_l\}$. Then, for any integer l, a sequence of indices $\{\mathbf{i}_1, \ldots, \mathbf{i}_l\}$, and an index $\mathbf{r} = (r_1, \ldots, r_l) \in \{1, \ldots, m\}^l$, we can define a function and a number. The function is

$$A(y; \mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l, \mathbf{r}) = \prod_{\omega=1}^l C^Y_{\mathbf{i}_\omega, r_\omega}(y), \tag{29}$$

where $C^Y_{\mathbf{i}_\omega, r_\omega}(y)$ given in (25) depends only on the model coefficients and their derivatives.

The key to deriving the expansion coefficients lies in calculating the conditional expectation of the product of iterated Itô integrals, specifically,

$$\mathbb{E}\left[\prod_{\omega=1}^l \mathbb{I}_{\mathbf{i}_\omega}(t) \,\middle|\, W(t) = x\right]. \tag{30}$$

Lemma 2 in the Appendix gives explicit recursive formulas for evaluating (30), which are crucial for obtaining the expansion coefficients.

Now we are ready to present the main theorem. The expansion coefficients are reduced to linear combinations of the integrals $I(f(\cdot), \cdot)$ defined in (27), where the combination of coefficients can be precomputed in advance. Thus, we only need to compute the integrals $I(f(\cdot), \cdot)$.

Theorem 1. *In the expansion* (26)*, the leading term is given by*

$$\Omega_0\big(y; f(\cdot)\big) = \int_{\mathbb{R}^m} f(z)\phi(z)\, \mathrm{d}z. \tag{31}$$

The other expansion coefficients $\Omega_k\big(y; f(\cdot)\big)$ *for* $k \geq 1$ *admit the representation*

$$\Omega_k\big(y; f(\cdot)\big) = \sum_{l=1}^k \frac{1}{l!} \sum_{\substack{\mathbf{j}=(j_1, j_2, \ldots, j_l) \\ \in \mathcal{S}_k^l}} \sum_{\substack{\mathbf{i}_\omega \in \mathcal{M}_{j_\omega + 1} \\ \omega = 1, \ldots, l}} \sum_{\mathbf{r} \in \{1,2,\ldots,m\}^l} A(y; \mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l, \mathbf{r}) B(f(\cdot); \mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l, \mathbf{r}), \tag{32}$$

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where $\mathcal{S}_k^l$ and $\mathcal{M}_j$ are defined by (28) and (24), respectively. The function A is defined by (29), and the number B is given by

$$B(f(\cdot);\ddot{\mathbf{i}},\mathbf{r}) = \sum_{0\le\mathbf{a}\le\lfloor\mathbf{c}_{\ddot{\mathbf{i}}}/2\rfloor} \frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}})-|\mathbf{a}|)!}\cdot I\big(f(\cdot),\mathbf{c}_{\ddot{\mathbf{i}}}-2\mathbf{a}+\mathbf{b}_{\mathbf{r}}\big). \tag{33}$$

Here $I(f(\cdot),\cdot)$ is the integral defined by (27) involving the function $f(\cdot)$. For ease of exposition, we let $\ddot{\mathbf{i}}=\mathbf{i}_1\wedge\cdots\wedge\mathbf{i}_l$ denote the concatenated index vector, and $\ell(\ddot{\mathbf{i}})$ is defined by (A2), representing the total dimensionality of the concatenated vector $\ddot{\mathbf{i}}$; $\mathbf{c}_{\ddot{\mathbf{i}}}\in\mathbb{Z}_+^m$ is defined by (A1), $\mathbf{b}_{\mathbf{r}}=\sum_{\omega=1}^l e_{r_\omega}$, and $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$ are constant coefficients recursively defined by (A4).

Remark 4. It is worth mentioning that by replacing the iterated Itô integrals in (30) with iterated Stratonovich integrals, the conditional expectations of products of iterated Stratonovich integrals become the building blocks of the pathwise expansion proposed in [26]. Appendix A of [26] provides an effective algorithm for computing these conditional expectations with three major steps, which are further elaborated in Section 4 of [27] and Section 4 of [28]. In contrast to the algorithms described over several pages in [26, 27, 28], our approach avoids the use of Stratonovich integrals, eliminating the need for algorithms that convert the multiplication of iterated Stratonovich integrals to iterated Itô integrals. In addition, the formula in our Lemma 2 is explicit and more straightforward to implement.

Note that both (31) and (32) (related to (27)) involve multivariate integrals. However, compared with (13) and (14), a key result of the quasi-Lamperti transform is that the multivariate normal density here is uncorrelated, allowing it to be factored into a product of its univariate counterparts. The same property holds for the associated multivariate Hermite polynomials. Consequently, when the function $f(z)$ depends on only one component or can be decomposed into a sum of products of its components, these multivariate integrals effectively reduce to one-dimensional integrals, significantly simplifying the computation. Specifically, for certain functions—such as the Dirac delta function, Hermite polynomials, indicator functions, and vanilla option payoff functions—the multivariate integrals in (31) and (32) (related to (27)) can be simplified to explicit analytical formulas, eliminating the need for direct integration.

In the next section, we provide explicit formulas for computing the multivariate integrals in (31) and (32) (related to (27)) for these special functions. These results are useful for deriving closed-form expansions for CDFs, European option prices, and transition densities.

4. Explicit expansion formulas for marginal CDFs, European option prices, and transition densities

To demonstrate how to apply Theorem 1, we discuss three important special cases in this section. By specifying the function f in the theorem to be an indicator function, a vanilla option payoff function, or a Dirac delta function, our method produces explicit expansion formulas for marginal CDFs, European option prices, and the transition density of multivariate diffusion models.

4.1. The marginal CDF

In this subsection, we obtain an expansion for the marginal CDF of the first state variable. To the best of our knowledge, this expansion formula for the marginal CDF is new to the

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literature. Specifically, the marginal CDF is given by

$$\begin{aligned}\mathbb{P}\big[X_1(t') < x_1' \,\big|\, X(t) = x\big] &= \mathbb{P}\left[L_{11}\frac{X_1(t') - x_1}{\sqrt{t'-t}} < L_{11}\frac{x_1' - x_1}{\sqrt{t'-t}} \,\middle|\, X(t) = x\right] \\ &= \mathbb{E}\left[f\left(\frac{Y(t') - y}{\sqrt{t'-t}}\right) \,\middle|\, Y(t) = y\right], \end{aligned} \tag{34}$$

where $L_{11} > 0$ is the element in the first row and first column of the matrix L in (16). Throughout this subsection and the next, we assume without loss of generality that $\sigma^X(x)$ is lower triangular, which implies that $L = (\sigma^X(x))^{-1}$ is also lower triangular with $L_{11} = 1/\sigma_{11}^X(x)$.

Given the transformations $y = Lx$ and $y' = Lx'$, we define $\gamma = (y' - y)/\sqrt{t'-t}$, with its first component specifically given by $\gamma_1 = L_{11}\frac{x_1' - x_1}{\sqrt{t'-t}} = \frac{x_1' - x_1}{\sigma_{11}^X(x)\sqrt{t'-t}}$. The function f is defined as $f(z) = \mathbf{1}_{z_1 < \gamma_1}$. Here, the subscript 1 for a vector denotes its first element.

Comparing with (22), we can derive an expansion for the marginal CDF (34) by plugging this indicator function into Theorem 1. Specifically, for $f(z) = \mathbf{1}_{z_1 < \gamma_1}$, the multivariate integral in (31) is given by

$$\Omega_0\big(y; f(\cdot)\big) = \int_{\mathbb{R}^m} f(z)\phi(z)\,\mathrm{d}z = \int_{\mathbb{R}} \mathbf{1}_{z_1 < \gamma_1}\phi(z_1)\,\mathrm{d}z_1 = \Phi(\gamma_1), \tag{35}$$

where $\Phi(\cdot)$ is the one-dimensional standard normal CDF. The multivariate integral in (32) (related to (27)) is given by

$$\int_{\mathbb{R}^m} \mathbf{1}_{z_1 < \gamma_1} H_h(z)\phi(z)\,\mathrm{d}z = J_{h_1}(\gamma_1) \cdot \mathbf{1}_{\{h_i = 0, i = 2, \ldots, m\}}, \tag{36}$$

where the function $J_{h_1}(\gamma_1)$ is defined as

$$J_{h_1}(\gamma_1) = \int_{\mathbb{R}} \mathbf{1}_{z_1 < \gamma_1} H_{h_1}(z_1)\,\phi(z_1)\,\mathrm{d}z_1 = \mathbf{1}_{h_1 = 0} \cdot \Phi(\gamma_1) - \mathbf{1}_{h_1 > 0} \cdot H_{h_1 - 1}(\gamma_1)\phi(\gamma_1). \tag{37}$$

4.2. European call option price

In this subsection, we derive a price expansion for a European call option written on the first state variable. Throughout this subsection, we assume that X in (1) is defined under a risk-neutral measure. At the current time t, given $X(t) = x$, the price of the European contingent claim, whose payoff function is $(\mathrm{e}^{X_1(t')} - \mathrm{e}^a)^+$ maturing at t', is given by

$$\begin{aligned} C(t, x) &= \mathrm{e}^{-r\Delta}\,\mathbb{E}\big[(\mathrm{e}^{X_1(t')} - \mathrm{e}^a)^+ \,\big|\, X(t) = x\big] \\ &= \mathrm{e}^{-r\Delta}\,\mathbb{E}\left[\left(\mathrm{e}^{L_{11}^{-1}\sqrt{\Delta}\left(L_{11}\frac{X_1(t') - x_1}{\sqrt{t'-t}}\right) + x_1} - \mathrm{e}^a\right)^+ \,\middle|\, X(t) = x\right] \\ &= \mathrm{e}^{-r\Delta}\,\mathbb{E}\left[f\left(\frac{Y(t') - y}{\sqrt{t'-t}}\right) \,\middle|\, Y(t) = y\right], \end{aligned} \tag{38}$$

where r is the risk-free interest rate, $\Delta = t' - t$, $L_{11} = 1/\sigma_{11}^X(x) > 0$ is the element in the first row and first column of the matrix L in (16), $y = Lx$, and $y' = Lx'$. The function f in this subsection is given by

$$f(z) = \left(\mathrm{e}^{\sigma_{11}^X(x)\sqrt{\Delta}z_1 + x_1} - \mathrm{e}^a\right)^+, \tag{39}$$

where the subscript 1 for a vector denotes the first element of that vector.

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Comparing with (22), we can derive an expansion for the call option price (38) by plugging the function in (39) into Theorem 1. Specifically, the multivariate integral in (31) is given by

$$\begin{aligned}\Omega_0\big(y;f(\cdot)\big) &= \int_{\mathbb{R}^m} f(z)\phi(z)\,\mathrm{d}z = \int_{\mathbb{R}} \left(\mathrm{e}^{\sigma_{11}^X(x)\sqrt{\Delta}z_1+x_1} - \mathrm{e}^a\right)^+ \phi(z_1)\,\mathrm{d}z_1 \\ &= \mathrm{e}^{x_1+\frac{1}{2}(\sigma_{11}^X(x))^2\Delta}\,\Phi\,(d_2) - \mathrm{e}^a\Phi\,(d_1)\,, \end{aligned} \tag{40}$$

where $d_1 = \frac{x_1-a}{\sigma_{11}^X(x)\sqrt{\Delta}}$, $d_2 = d_1 + \sigma_{11}^X(x)\sqrt{\Delta}$, and $\Phi(\cdot)$ is the one-dimensional standard normal CDF. The multivariate integral in (32) (related to (27)) is given by

$$\begin{aligned}\int_{\mathbb{R}^m} f(z)H_h(z)\phi(z)\,\mathrm{d}z &= \int_{\mathbb{R}} \left(\mathrm{e}^{\sigma_{11}^X(x)\sqrt{\Delta}z_1+x_1} - \mathrm{e}^a\right)^+ H_{h_1}(z_1)\phi(z_1)\,\mathrm{d}z_1 \\ &= \left(\sigma_{11}^X(x)\sqrt{\Delta}\right)^{h_1} \mathrm{e}^{x_1+\frac{1}{2}(\sigma_{11}^X(x))^2\Delta}\cdot\Phi(d_2) \\ &\quad + \mathrm{e}^a \sum_{1\le i\le h_1-1} \left(\sigma_{11}^X(x)\Delta\right)^{h_1-i}(-1)^{i-1}H_{i-1}(d_1)\phi(d_1) = I_{h_1}. \end{aligned} \tag{41}$$

We can simply obtain the approximation of the put price using the put-call parity and the call price approximation.

4.3. The transition density function

In this subsection, we provide an expansion for the transition density function of the diffusion. Given $t' > t$, the transition density function of the diffusion X from $X(t) = x$ to $X(t') = x'$ admits the following expression (see e.g. [26, 35, 36]):

$$p_X(t', x' \mid t, x) = \mathbb{E}[\delta(X(t') - x') \mid X(t) = x], \tag{42}$$

where $\delta(\cdot)$ is the Dirac delta function. We can rewrite it using the Jacobian formula for the change of density as

$$p_X(t', x' \mid t, x) = \Delta^{-\frac{m}{2}}\mathbb{E}\left[\delta\left(\frac{X(t')-x}{\sqrt{\Delta}} - \frac{x'-x}{\sqrt{\Delta}}\right)\,\middle|\, X(t) = x\right] \tag{43}$$

$$= \Delta^{-\frac{m}{2}}\det(L)\,\mathbb{E}\left[\delta\left(\frac{Y(t')-y}{\sqrt{\Delta}} - \gamma\right)\,\middle|\, Y(t) = y\right], \tag{44}$$

where $y = Lx$, $y' = Lx'$, $\gamma = (y'-y)/\sqrt{\Delta}$, and $\Delta = t' - t$.

Comparing the conditional expectation in (43) and (44) with (22), we can specify the following function f to derive an expansion for the transition density function:

$$f(\cdot) = \delta(\,\cdot - \gamma). \tag{45}$$

Specifically, the multivariate integrals in (31) and (32) (related to (27)) are now given by

$$\Omega_0\big(y;f(\cdot)\big) = \int_{\mathbb{R}^m} \delta(z-\gamma)\phi(z)\,\mathrm{d}z = \phi(\gamma) \tag{46}$$

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and

$$\int_{\mathbb{R}^m} \delta(z-\gamma)H_{\mathbf{h}}(z)\phi(z)\,\mathrm{d}z = H_{\mathbf{h}}(\gamma)\phi(\gamma). \tag{47}$$

Plugging these into Theorem 1, together with (44) and (26), we can obtain an explicit recursive formula for the expansion of the transition density function. To save space here, we present the result in Appendix C; see (C1) for the complete expression.

Appendix C.1 says that this provides an alternative explicit expression for the expansion formula in [26] and [28]. However, unlike the formula presented in those works, the newly derived formula is explicitly expressed as a linear combination of Hermite polynomials. This form allows us to connect the expression to the Hermite expansion of [34] and [36]. By carefully rearranging the terms in the expansions, it is proved in Appendix C.2 that the density expansions from [26] and [34, 36] are equivalent. The following theorem summarizes these results.

Theorem 2. (Equivalence theorem.) *For a multivariate diffusion X as defined in* (1)*, the pathwise expansion* (3.21) *in* [26] *and the Hermite expansion* (32) *in* [34] *(or equivalently* (22) *in* [36] *with the choice of* $\mu_0 = 0$*) have the same formula.*

5. Applications in risk management and derivatives pricing with numerical experiments

This section presents two applications of the explicit expansion formulas derived above, which yield results that are new to the literature. The first application focuses on computing the VaR for a portfolio that incorporates both a stochastic risk premium and stochastic volatility factors. By using the approximation of the marginal CDF, we compute the VaR for a three-dimensional model (which may be nonaffine) that includes both factors. The second application involves pricing forward-starting call options under general stochastic volatility models, which may be nonaffine. The closed-form approximate formula is derived by integrating the transition density with the European call option price. To the best of our knowledge, the VaR computation using the approximate marginal CDF in three-dimensional (possibly nonaffine) models and the closed-form approximate formula for forward-starting option prices under general stochastic volatility (possibly nonaffine) models are entirely new to the literature. Numerical results show that the approximate formulas for density, CDF, and option price are both highly accurate and computationally efficient.

5.1. VaR for multi-asset portfolio losses

In this subsection, we use our approximation formulas to calculate the VaR for portfolio losses in a continuous-time financial market. VaR plays a crucial role in risk management, providing a clear, quantitative benchmark for assessing risk exposure. Moreover, it enables investors to make more informed decisions, helping them optimize portfolios to better withstand market fluctuations.

Specifically, we assume the presence of one riskless bond and $\mathcal{N}$ risky stocks. The risk-free interest rate at time t is r_t, and the dynamics of the stock prices S_i $(i = 1, \ldots, \mathcal{N})$ follow diffusion processes given by

$$\mathrm{d}S_{it}/S_{it} = a_i(\boldsymbol{x}_t)\,\mathrm{d}t + \sum_{j=1}^{\mathcal{N}} b_{ij}(\boldsymbol{x}_t)\,\mathrm{d}\mathcal{B}_{jt},$$

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where $\boldsymbol{\mathcal{B}}_t = (\mathcal{B}_{jt})_{\mathcal{N}\times 1}$ is a standard $\mathcal{N}$-dimensional Brownian motion, and the drift $\boldsymbol{a}_t = (a_i(\boldsymbol{x}_t))_{\mathcal{N}\times 1}$ and volatility $\boldsymbol{b}_t = (b_{ij}(\boldsymbol{x}_t))_{\mathcal{N}\times\mathcal{N}}$ are assumed to be deterministic functions of a $\mathcal{K}$-dimensional stochastic state variable $\boldsymbol{x}_t$. Consider a portfolio that invests a proportion π_i of wealth in the risky asset i for $1 \le i \le \mathcal{N}$. Let M_t be the portfolio value at time t. Then, a value of $\pi_i M_t$ will be invested in stock i for all $i = 1, \ldots, \mathcal{N}$, and the remaining value, $1 - \sum_{i=1}^{\mathcal{N}} \pi_i$, will be invested in the riskless bond. Consequently, the portfolio value M_t evolves according to

$$\begin{aligned} \mathrm{d}M_t &= M_t r(\boldsymbol{x}_t)\left(1 - \sum_{i=1}^{\mathcal{N}} \pi_i\right)\mathrm{d}t + \sum_{i=1}^{\mathcal{N}} \frac{M_t \pi_i}{S_{it}}\,\mathrm{d}S_{it} \\ &= r(\boldsymbol{x}_t) M_t\,\mathrm{d}t + \boldsymbol{\pi}^\top\big(\boldsymbol{a}(\boldsymbol{x}_t) - r(\boldsymbol{x}_t)\big) M_t\,\mathrm{d}t + M_t \boldsymbol{\pi}^\top \boldsymbol{b}(\boldsymbol{x}_t)\,\mathrm{d}\boldsymbol{\mathcal{B}}_t. \end{aligned}$$

Suppose that the vector $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_{\mathcal{N}})^\top$ remains constant over a time horizon T. Investors are interested in evaluating the VaR of such a portfolio at level $q \in (0, 1)$, denoted by VaR_T^q. This quantity is defined as

$$\mathrm{VaR}_T^q = \max\{y : \mathbb{P}(M_0 - M_T \ge y)\} \ge q.$$

In words, VaR_T^q is the maximum value such that the probability of the portfolio's loss $(M_0 - M_T)$ exceeding this value is at least q. We use 'maximum' instead of 'supremum' because M_T is a continuous random variable. Furthermore, we have

$$\mathbb{P}\big(M_0 - M_T \ge \mathrm{VaR}_T^q\big) = q.$$

Let $X_{1t} = \log(M_t)$. Then it is easy to see that $M_T = \exp(X_{1T})$. Denote by

$$F_{X_{1T}}(x) = \mathbb{P}\big(X_{1T} \le x \,\big|\, X_{10}\big)$$

the marginal CDF of X_{1T} with the initial $X_{10} = \log(M_0)$. Using this notation, the VaR at level q can be represented as

$$\mathrm{VaR}_T^q = \exp(X_{10}) - \exp\big(F_{X_{1T}}^{-1}(q)\big).$$

Our expansion approach produces approximations to the CDF $F_{X_{1T}}(x)$. Combining these with some numerical root-finding algorithms (e.g. Newton's method), we can approximately solve for $F_{X_{1T}}^{-1}(q)$ and thereby obtain VaR_T^q.

Let us investigate one example to numerically test the accuracy and effectiveness of our approximation approach. In addition to the log-portfolio value process X_{1t}, this example involves a two-dimensional state variable $\boldsymbol{x}_t = (X_{2t}, X_{3t})$, in which X_{2t} and X_{3t} represent two factors for determining the risk premiums and stochastic volatility of the stocks at time t, respectively. Assume $r(\boldsymbol{x}_t) = r$ in the example. In other words, the bond investment offers a constant interest return r over time. In addition, the risk premium $\boldsymbol{a}(\boldsymbol{x}_t) - r(\boldsymbol{x}_t)$ is linearly dependent on the risk factor X_{2t}:

$$\boldsymbol{a}(\boldsymbol{x}_t) - r(\boldsymbol{x}_t) = X_{2t} \cdot \boldsymbol{\eta}$$

for a constant $\boldsymbol{\eta} \in \mathbb{R}^{\mathcal{N}}$. The volatility matrix is given by $\boldsymbol{b}(\boldsymbol{x}_t) = \sqrt{X_{3t}} \cdot \boldsymbol{\sigma}$, where $\boldsymbol{\sigma}$ is a constant coefficient matrix.

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Under this setup, the portfolio value process follows

$$\mathrm{d}M_t = rM_t\,\mathrm{d}t + (\boldsymbol{\pi}^\top \cdot \boldsymbol{\eta})X_{2t}M_t\,\mathrm{d}t + M_t\sqrt{X_{3t}}\,(\boldsymbol{\pi}^\top \cdot \boldsymbol{\sigma})\,\mathrm{d}\boldsymbol{\mathcal{B}}_t. \tag{48}$$

For notational simplicity, we write $\theta_1 = \boldsymbol{\pi}^\top \cdot \boldsymbol{\eta}$. Meanwhile, we know that there must exist a constant σ_1 and a one-dimensional Brownian motion W_{1t} such that $\sigma_1\,\mathrm{d}W_{1t} \overset{\mathrm{d}}{=} \boldsymbol{\pi}^\top \boldsymbol{\sigma}\,\mathrm{d}\boldsymbol{\mathcal{B}}_t$. Since we are interested in the VaR of M_t, a quantity related to the distributional law of $\boldsymbol{\pi}^\top \boldsymbol{\sigma}\,\mathrm{d}\boldsymbol{\mathcal{B}}_t$, we can replace it with $\sigma_1\,\mathrm{d}W_{1t}$ in the dynamics (48). Using Itô's formula, we have

$$\mathrm{d}X_{1t} = \left(r + \theta_1 X_{2t} - \tfrac{1}{2}\sigma_1^2 X_{3t}\right)\mathrm{d}t + \sigma_1\sqrt{X_{3t}}\,\mathrm{d}W_{1t}. \tag{49}$$

To complete the model, assume that the state variables $\boldsymbol{x}_t = (X_{2t}, X_{3t})$ follow

$$\mathrm{d}X_{2t} = \kappa_2 \cdot (\theta_2 - X_{2t}) \cdot X_{2t}\,\mathrm{d}t + \sigma_2 \cdot (\rho_{12}\,\mathrm{d}W_{1t} + \bar{\rho}_{22}\,\mathrm{d}W_{2t}) \tag{50}$$

and

$$\mathrm{d}X_{3t} = \kappa_3 \cdot (\theta_3 - X_{3t})\,\mathrm{d}t + \sigma_3 X_{3t}^{\beta} \cdot (\rho_{13}\,\mathrm{d}W_{1t} + \rho_{23}\,\mathrm{d}W_{2t} + \bar{\rho}_{33}\,\mathrm{d}W_{3t})\,. \tag{51}$$

Here (W_{1t}, W_{2t}, W_{3t}) is a standard three-dimensional Brownian motion. The quantities ρ_{12}, $\bar{\rho}_{22}$, ρ_{13}, ρ_{23}, and $\bar{\rho}_{33}$ define the correlations among these three processes. Specifically, $\bar{\rho}_{22} = \sqrt{1-\rho_{12}^2}$ and

$$\bar{\rho}_{33} = \sqrt{1-\rho_{13}^2-\rho_{23}^2}.$$

In our model, the risk premium process X_2 follows an Ornstein–Uhlenbeck process characterized by mean-reversion speed κ_2, long-term mean θ_2, and volatility σ_2. The mean-reverting behavior of X_2 reflects the tendency of risk premiums to revert to a long-term average, capturing shifting market expectations and changes in risk appetite. The volatility process X_3 is also mean-reverting, with nonlinearity controlled by the parameter β. When $\beta = \frac{1}{2}$, the volatility follows a square-root process, commonly referred to as the SR-SV-$\frac{1}{2}$ model. Here, SR denotes stochastic return (or stochastic risk premium) while SV-$\frac{1}{2}$ indicates the square-root specification for stochastic volatility. For $\beta = 1$, the SR-SV-1 model represents a linear relationship between volatility and X_3. When $\beta \in \left(\frac{1}{2}, 1\right)$, the SR-SV-$\beta$ model provides a more flexible, nonlinear volatility specification, capable of capturing complex dynamics such as asymmetric responses to shocks and volatility clustering.

Table 1 presents the VaR estimates for the portfolio losses, considering stochastic risk premium and stochastic volatility. These values are calculated using three different models, SR-SV-$\frac{1}{2}$, SR-SV-β, and SR-SV-1, across two confidence levels, $q = 0.01$ and $q = 0.05$. The results are provided for various time horizons, including daily, weekly, biweekly, monthly, quarterly, and semi-annually, i.e. $T = 1/252, 1/52, 1/26, 1/12, 1/4, 1/2$. These time horizons capture various trading or observation intervals. For the parameter values, the reader is referred to the empirical literature, such as [4, 31].

For each model, the 'MC' values are obtained from Monte Carlo simulations, which serve as the benchmark. The number of simulation trials is 10 million, and the number of time steps is 25 200 per year. The 'Appr.' values are obtained through analytical approximations using the model's specified parameters. The relative error, RE, between the two methods is shown in the last row for each time horizon, calculated as the percentage difference between the approximate and MC values, i.e. $\mathrm{RE} = |\mathrm{Appr.} - \mathrm{MC}|/\mathrm{MC}$.

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TABLE 1. VaR for portfolio losses with stochastic risk premium and stochastic volatility.

				$q = 0.01$			
Model	T	1/252	1/52	1/26	1/12	1/4	1/2
SR-SV-$\frac{1}{2}$	MC	4.5753	9.9146	13.8358	19.8804	32.2889	42.2426
	Appr.	4.5773	9.9162	13.8382	19.8904	32.5775	42.0200
	RE	0.04%	0.02%	0.02%	0.04%	0.10%	0.53%
SR-SV-β	MC	3.8948	8.3916	11.6773	16.6799	26.8425	35.0285
	Appr.	3.8938	8.3953	11.6744	16.7048	26.8671	34.9948
	RE	0.03%	0.04%	0.00%	0.04%	0.13%	0.10%
SR-SV-1	MC	4.0985	8.7778	12.1377	17.2274	24.4159	35.6338
	Appr.	4.0995	8.7717	12.1361	17.2323	24.4016	35.2737
	RE	0.03%	0.07%	0.01%	0.03%	0.05%	1.01%
				$q = 0.05$			
Model	T	1/252	1/52	1/26	1/12	1/4	1/2
SR-SV-$\frac{1}{2}$	MC	3.2204	6.9443	9.6559	13.8292	22.4011	29.4897
	Appr.	3.2211	6.9443	9.6591	13.8317	22.3646	29.0799
	RE	0.02%	0.01%	0.03%	0.02%	0.16%	1.39%
SR-SV-β	MC	2.7409	5.8733	8.1424	11.5577	18.4573	23.9925
	Appr.	2.7403	5.8757	8.1455	11.5788	18.4233	23.4358
	RE	0.03%	0.04%	0.02%	0.03%	0.18%	2.32%
SR-SV-1	MC	2.8972	6.1836	8.5632	12.1384	19.2776	25.0711
	Appr.	2.8958	6.1892	8.5561	12.1358	19.2712	24.8071
	RE	0.05%	0.06%	0.08%	0.10%	0.03%	1.05%

Note: The upper and lower panels correspond to quantile levels at $q = 0.01$ and $q = 0.05$, respectively. RE denotes the relative error computed via RE $= |\text{Appr.} - \text{MC}|/\text{MC}$, where 'MC' is generated by Monte Carlo simulations and 'Appr.' is obtained through the approximate formulas derived in this paper. For all the models, in the log-wealth process we set $r = 0.04$, $X_{10} = \log(100)$, $\eta = 1$, and $\sigma_1 = 1$. In the stochastic risk premium process, the parameters are $\kappa_2 = 2$, $X_{20} = \theta_2 = 0.1$, $\sigma_2 = 0.2$, $\rho_{12} = -0.2$, and $\rho_{23} = 0$. For the stochastic volatility process, three sets of parameter values are considered based on different specifications of β. Under the SV-1/2 specification, we set $\kappa_3 = 5.07$, $X_{30} = \theta_3 = 0.0457$, $\sigma_3 = 0.48$, $\rho_{13} = -0.767$, $\rho_{23} = 0$, and $\beta = 1/2$. Under the SV-1 specification, we set $\kappa_3 = 1.62$, $X_{30} = \theta_3 = 0.074$, $\sigma_3 = 2.204$, $\rho_{13} = -0.754$, $\rho_{23} = 0$, and $\beta = 1$. Under the SV-β specification, we set $\kappa_3 = 4.103$, $X_{30} = \theta_3 = 0.0451$, $\sigma_3 = 0.858$, $\rho_{13} = -0.76$, $\rho_{23} = 0$, and $\beta = 0.655$.

The results in Table 1 reveal how the VaR estimates change with different models, quantile levels, and time horizons, illustrating the sensitivity of the portfolio's risk profile to these factors. One key observation is the effect of the time horizon on the VaR estimates. As the time horizon increases from 1/252 to 1/2, the VaR values rise for all models and quantile levels ($q = 0.01$ and $q = 0.05$). This is to be expected, as longer time horizons account for greater uncertainty and higher potential losses. Comparison of the two quantile levels reveals that the VaR values for $q = 0.01$ (1%) are consistently higher than those for $q = 0.05$ (5%), reflecting the more extreme loss scenario associated with the 1% quantile.

The approximate values are very close to the Monte Carlo results (benchmark values), with relative errors typically remaining below 0.2% for most time horizons and confidence levels. In particular, for the SR-SV-$\frac{1}{2}$ model, the approximate values are in near-perfect alignment with the Monte Carlo results, and the relative errors remain small across both confidence levels

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($q = 0.01$ and $q = 0.05$), except for $T = 1/2$ and $q = 0.05$, for which the relative error reaches 1.39%. A similar pattern is observed for the SR-SV-β model, where the approximate values again closely match the Monte Carlo results, with relative errors mostly below 0.2%, except for $T = 1/2$ and $q = 0.05$, for which the relative error reaches a slightly higher level, 2.32%. For the SR-SV-1 model, the approximation remains accurate, and the relative errors are less than 0.1% for most time horizons. When $T = 1/2$, the relative errors are around 1% for both confidence levels.

Overall, Table 1 demonstrates that the approximate formulas provide highly accurate VaR estimates compared to the Monte Carlo simulations, with very small relative errors across all models and time horizons. This indicates that the approximation methods provide an accurate and efficient alternative way of calculating VaR in portfolios with stochastic risk premiums and stochastic volatility.

5.2. Pricing forward-starting options

This section explores another application of our expansion method in the context of complex derivative pricing, using forward-starting options as an example. In a forward-starting option contract, the strike price is determined by the future price of the underlying asset. Such derivatives are widely employed in risk management and portfolio optimization owing to their flexibility, making them a popular choice for both hedging and speculating on future price movements.

Consider the following model for the underlying asset price with one stochastic volatility factor. The state variable $X(t) = (X_1(t), X_2(t))$ is a two-dimensional diffusion process, where the first component $X_1(t)$ represents the log-return of the underlying asset and the second component $X_2(t)$ is the instantaneous variance of the log-return process. Under the risk-neutral measure $\mathbb{Q}$, the dynamics of $(X_1(t), X_2(t))$ are governed by

$$\mathrm{d}X_1(t) = \left(r - \frac{1}{2}X_2(t)\right)\mathrm{d}t + \sqrt{X_2(t)}\,\mathrm{d}W_1(t), \tag{52}$$

$$\mathrm{d}X_2(t) = \kappa(\alpha - X_2(t))\,\mathrm{d}t + \sigma X_2^{\beta}\left(\rho\,\mathrm{d}W_1(t) + \sqrt{1-\rho^2}\,\mathrm{d}W_2(t)\right). \tag{53}$$

Here, r is the risk-free rate and ρ is the constant correlation parameter between the return and variance processes. The variance process X_2 exhibits mean reversion to its long-term mean α, with κ being the speed of mean reversion; σ represents the volatility of volatility, and β is the elasticity of the local volatility function, satisfying $1/2 \le \beta \le 1$; κ, α, σ, and β are all assumed to be nonnegative constants.

The process in (52) and (53) defines a broad class of models. When $\beta = 1/2$, the variance process X_2 is the affine square-root model of [15]. To ensure that the volatility cannot reach zero with positive probability, we require $2\kappa\alpha \ge \sigma^2$. This process along with the log-return process X_1, called the SV-1/2 model, corresponds to the affine stochastic volatility model of [18]. When $\beta = 1$ or $\beta \in (1/2, 1)$, the variance processes correspond to the nonaffine continuous-time GARCH model [16, 30] and the CEV model, respectively. The SV-β and SV-1 models refer to those with CEV [20] and GARCH specifications of the variance. Nonaffine models lack closed-form option price formulas and require numerical methods, such as finite difference or Monte Carlo simulations. However, they often outperform affine models empirically [4, 20, 31].

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Given $0 \le t < t^* < T$, the payoff function of a forward-starting option is

$$\left(\mathrm{e}^{X_1(T)} - \mathrm{e}^{X_1(t^*)}\right)^+. \tag{54}$$

Assuming that we know the model's transition density $p(t', x' \mid t, x)$, the price of the forward-starting option, $C_{FWS}(t, x)$, is given by the conditional expectation

$$\begin{aligned} C_{FWS}(t, x) &= \mathrm{e}^{-r(T-t)}\, \mathbb{E}\left[\left(\mathrm{e}^{X_1(T)} - \mathrm{e}^{X_1(t^*)}\right)^+ \,\middle|\, X(t) = x\right] \\ &= \mathrm{e}^{-r(T-t)} \int \mathbb{E}\left[\left(\mathrm{e}^{X_1(T)} - \mathrm{e}^{x_1^*}\right)^+ \,\middle|\, X(t^*) = x^*\right] \cdot p(t^*, x^* \mid t, x)\, \mathrm{d}x^*. \end{aligned} \tag{55}$$

Thus, the forward-starting option price in (55) is the integral of the product of the European option price (the conditional expectation) and the transition density. Therefore, using the approximations for both, we obtain a closed-form approximation formula for (55). It is worth noting that [23] provides a closed-form pricing formula (essentially involving a two-dimensional integral) for the affine SV-1/2 model.

We perform numerical experiments using the approximation formulas given by the European option price and the transition density. Table 2 presents the numerical performance results of the forward-starting option price approximations for different models (SV-1/2, SV-β, and SV-1) under various forward-starting dates t^* (weekly, biweekly, and monthly) and maturity periods $T - t^*$ (monthly, quarterly, and semi-annually). Each row corresponds to a specific combination of model, t^*, and $T - t^*$, and provides the following details. The first column, 'Model', indicates the three stochastic volatility models considered, which are SV-1/2, SV-β, and SV-1. The second and third columns, t^* and $T - t^*$, represent the time t^* at which the strike price of the forward-starting option is set and the time remaining to maturity after t^*, respectively.

The 'MC' column shows the forward-starting option price obtained from Monte Carlo simulations, which serves as the benchmark for comparison. The columns labeled '99% CI L' and '99% CI U' represent the lower and upper bounds, respectively, of the 99% confidence interval (CI) for the Monte Carlo price, providing a measure of the statistical uncertainty in the Monte Carlo estimate. The number of simulated sample paths is 10 million, and the number of time steps is 25 200 per year. The 'Appr.' column presents the price of the forward-starting option calculated using the closed-form approximation method proposed in this paper. The last column, 'RE', shows the relative error between the approximation price and the Monte Carlo price, i.e. RE = |Appr. − MC|/MC, expressed as a percentage. This value indicates the accuracy of the approximation method compared to the Monte Carlo results.

The results in Table 2 demonstrate that the proposed approximation yields highly accurate prices, with relative errors generally close to 0% for all three models. Overall, the approximation performs well across all test cases, showing minimal deviation from the Monte Carlo benchmark and suggesting that the closed-form method provides an accurate and efficient alternative to Monte Carlo simulations.

6. Concluding remarks

This paper presents a unified framework for deriving explicit expansion formulas for transition densities, CDFs, and European option prices in multivariate diffusion models. To develop such a framework, we introduce the quasi-Lamperti transform, which uses the diffusion matrix at the initial time, simplifying subsequent calculations. A key contribution of this work is

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TABLE 2. Numerical performance results for approximations of the forward-starting option prices.

Model	t^*	$T-t^*$	MC	99% CI L	99% CI U	Appr.	RE
SV-1/2	1/52	1/12	3.7853	3.7808	3.7899	3.7861	0.02%
	1/52	1/4	6.7346	6.7267	6.7424	6.7375	0.04%
	1/52	1/2	9.7623	9.7509	9.7737	9.7645	0.02%
	1/26	1/12	3.7786	3.7740	3.7831	3.7769	0.05%
	1/26	1/4	6.7244	6.7166	6.7323	6.7262	0.03%
	1/26	1/2	9.7533	9.7418	9.7648	9.7588	0.06%
	1/12	1/12	3.7589	3.7547	3.7631	3.7580	0.02%
	1/12	1/4	6.7015	6.6937	6.7093	6.7033	0.03%
	1/12	1/2	9.7259	9.7146	9.7373	9.7485	0.23%
SV-β	1/52	1/12	3.2640	3.2602	3.2677	3.2655	0.05%
	1/52	1/4	5.8480	5.8414	5.8547	5.8487	0.01%
	1/52	1/2	8.5343	8.5245	8.5441	8.5207	0.16%
	1/26	1/12	3.2594	3.2556	3.2632	3.2611	0.05%
	1/26	1/4	5.8435	5.8369	5.8502	5.8442	0.01%
	1/26	1/2	8.5320	8.5222	8.5419	8.5244	0.09%
	1/12	1/12	3.2502	3.2463	3.2540	3.2524	0.07%
	1/12	1/4	5.8338	5.8273	5.8403	5.8353	0.03%
	1/12	1/2	8.5225	8.5126	8.5324	8.5320	0.11%
SV-1	1/52	1/12	3.4566	3.4524	3.4608	3.4569	0.01%
	1/52	1/4	6.1849	6.1771	6.1927	6.1820	0.05%
	1/52	1/2	9.0054	8.9947	9.0160	8.9997	0.06%
	1/26	1/12	3.4542	3.4501	3.4583	3.4548	0.02%
	1/26	1/4	6.1841	6.1766	6.1915	6.1794	0.08%
	1/26	1/2	9.0028	8.9923	9.0133	8.9985	0.05%
	1/12	1/12	3.4513	3.4470	3.4556	3.4505	0.02%
	1/12	1/4	6.1781	6.1708	6.1854	6.1741	0.06%
	1/12	1/2	8.9970	8.9862	9.0077	8.9958	0.01%

Note: The t^* and $T-t^*$ columns represent the forward-starting date and the remaining maturity period, respectively. The last column, RE, displays the relative error computed via $\text{RE} = |\text{Appr.} - \text{MC}|/\text{MC}$, where 'MC' is generated by Monte Carlo simulations and 'Appr.' is obtained through the approximate formulas derived in this paper. The columns '99% CI L' and '99% CI U' represent the lower and upper bounds, respectively, of the 99% confidence interval (CI) for the Monte Carlo price. For all three models, the initial values of the log stock price and the volatility are $X_{10} = \log(100)$ and $X_{20} = \theta$. The parameter vector is denoted by $(r, \beta, \kappa, \theta, \sigma, \rho)$. For the SV-1/2 model, it is (0.04, 0.5, 3.0, 0.1, 0.25, −0.8). For the SV-β model, it is (0.04, 0.879, 4.202, 0.073, 0.471, −0.704). For the SV-1 model, it is (0.04, 1, 3.464, 0.082, 0.292, −0.811).

the derivation of explicit formulas for the conditional expectation of the pathwise Taylor expansion, leveraging explicit expressions for the conditional expectation of the product of iterated Itô integrals. This provides a new and generalizable approach to obtaining closed-form expressions for conditional expectations, addressing a fundamental challenge in the literature. Using our main result, we establish the equivalence between the pathwise expansion of [26] and the Hermite expansion of [34, 36], unifying them under the Hermite expansion method. This insight clarifies the connections between existing techniques and simplifies practical implementation.

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We apply our results to two financial problems: (i) the derivation of closed-form expansion formulas for forward-starting options under general stochastic volatility models (which may be nonaffine) and (ii) computation of the VaR for a portfolio in three-dimensional (possibly nonaffine) models incorporating both stochastic risk premium and volatility factors, using the expansion formulas for the marginal CDF. To the best of our knowledge, these two applications are new to the literature. Numerical experiments confirm the accuracy and efficiency of our approach.

Beyond these applications, our method provides a powerful tool for small-time approximations of functionals of multivariate diffusion processes, offering promising directions for future research in asset pricing and statistical estimation.

Appendix A. Explicit formula for the conditional expectation of the product of iterated Itô integrals

In this appendix, we present the lemma that calculates the conditional expectation of the product of the iterated Itô integrals in (30). Before stating the results, we introduce some notation.

For an index $\mathbf{i} = (i_1, \ldots, i_n) \in \{0, 1, \ldots, m\}^n$, define $c_{\mathbf{i}}(\alpha)$ to be the counter of a particular value $\alpha \in \{0, 1, \ldots, m\}$ in $\mathbf{i}$, that is,

$$c_{\mathbf{i}}(\alpha) = \sum_{k=1}^{n} \mathbf{1}_{\{i_k = \alpha\}}.$$

For instance, if $\mathbf{i} = (1, 1)$, then $c_{\mathbf{i}}(1) = 2$. Furthermore, define a new vector

$$\mathbf{c}_{\mathbf{i}} = (c_{\mathbf{i}}(1), \ldots, c_{\mathbf{i}}(m)). \tag{A1}$$

In the previous example, we know that $\mathbf{c}_{(1,1)} = (2, 0, \ldots, 0)$.

This notation can be extended to the concatenation of several index vectors. Consider two indices $\mathbf{i}$ and $\mathbf{j}$, where $\mathbf{i}$ and $\mathbf{j}$ may have different dimensionalities. Define a concatenation operation between these two vectors such that $\mathbf{i} \wedge \mathbf{j}$ is a new index vector obtained by putting $\mathbf{j}$ at the end of $\mathbf{i}$. It is easy to see that for any sequence of indices $\{\mathbf{i}_1, \ldots, \mathbf{i}_l\}$, the norm of the concatenated index vector is given by $\|\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l\| = \sum_{j=1}^{l} \|\mathbf{i}_j\|$. Meanwhile, $c_{\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l}(\alpha) = \sum_{j=1}^{l} c_{\mathbf{i}_j}(\alpha)$ for any given α and thus $\mathbf{c}_{\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l} = \sum_{j=1}^{l} \mathbf{c}_{\mathbf{i}_j}$. In addition, we let $\ell(\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l)$ represent the total dimensionality of the concatenated vector $\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l$. Clearly, $\ell(\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l)$ is equal to the sum of the dimensionalities of all the $\mathbf{i}_j$, and we have

$$\ell(\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l) = c_{\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l}(0) + \sum_{\alpha=1}^{m} c_{\mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l}(\alpha) = \sum_{\omega=1}^{l} \left(c_{\mathbf{i}_\omega}(0) + \sum_{\alpha=1}^{m} c_{\mathbf{i}_\omega}(\alpha) \right). \tag{A2}$$

With this notation, we can present the explicit formula for the conditional expectation of the product of iterated Itô integrals as follows.

Lemma 2. *The conditional expectation* (30) *is a linear combination of Hermite polynomials. Specifically, for indices* $\{\mathbf{i}_1, \ldots, \mathbf{i}_l\}$*, letting* $\ddot{\mathbf{i}}$ *be the concatenation of these indices (i.e.* $\ddot{\mathbf{i}} = \mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l$*), the conditional expectation in* (30) *can be decomposed into*

$$\mathbb{E}\left[\prod_{\omega=1}^{l} \mathbb{I}_{\mathbf{i}_\omega}(t) \,\middle|\, W(t) = x \right] = \sum_{0 \le \mathbf{a} \le \lfloor \mathbf{c}_{\ddot{\mathbf{i}}}/2 \rfloor} \tilde{w}_{\mathbf{a}, \ddot{\mathbf{i}}} \cdot \left(\frac{\sqrt{t}^{\|\ddot{\mathbf{i}}\|}}{(\ell(\ddot{\mathbf{i}}) - |\mathbf{a}|)!} H_{\mathbf{c}_{\ddot{\mathbf{i}}} - 2\mathbf{a}}\left(\frac{x}{\sqrt{t}} \right) \right). \tag{A3}$$

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Note that $\mathbf{c}_{\ddot{\mathbf{i}}}$ *in the subscript of the sum is an m-dimensional vector (cf.* (A1)*), and* $\lfloor \mathbf{c}_{\ddot{\mathbf{i}}}/2 \rfloor$ *is a vector that is obtained by applying the operation of* $\lfloor \cdot/2 \rfloor$ *elementwise on* $\mathbf{c}_{\ddot{\mathbf{i}}}$*. In this sense, the sum in* (A3) *is taken over an m-dimensional index* $\mathbf{a} = (a_1, \ldots, a_m)$ *with* $|a| = a_1 + \cdots + a_m$*. Here* $\|\ddot{\mathbf{i}}\| = \sum_{j=1}^{l} \|\mathbf{i}_j\|$ *with the norm* $\|\mathbf{i}_j\|$ *defined in* (23)*, and* $\ell(\ddot{\mathbf{i}})$ *is defined in* (A2)*.*

The coefficient $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$ *is recursively determined as follows:* $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}} = \mathbf{1}_{\{\mathbf{a}=0\}}$ *if* $\ddot{\mathbf{i}} = \emptyset$ *or* $\{\mathbf{i}_1\}$*;* $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}} = 0$ *if* $\min(\mathbf{a}) < 0$ *or* $\max(2\mathbf{a} - \mathbf{c}_{\ddot{\mathbf{i}}}) > 0$*; and*

$$\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}} = \sum_{\omega_1=1}^{l} \tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}_{-\omega_1}} + \sum_{1 \le \omega_1 < \omega_2 \le l} \mathbf{1}_{\{(i_{\omega_1})_1 = (i_{\omega_2})_1 \neq 0\}} \tilde{w}_{\mathbf{a}-e_{(i_{\omega_1})_1},\ddot{\mathbf{i}}_{-\omega_1-\omega_2}}, \tag{A4}$$

where $\ddot{\mathbf{i}}_{-\omega_1}$ *means replacing the* ω_1*th component of* $\ddot{\mathbf{i}}$*, i.e.* $\mathbf{i}_{\omega_1} = \big((i_{\omega_1})_1, (i_{\omega_1})_2, \ldots, (i_{\omega_1})_{n_{\omega_1}}\big)$*, with* $-\mathbf{i}_{\omega_1} = \big((i_{\omega_1})_2, \ldots, (i_{\omega_1})_{n_{\omega_1}}\big)$ *in the set* $\ddot{\mathbf{i}}$*;* e_α *(for* $\alpha = 1, \ldots, m$*) is the m-dimensional vector in which the* α*th component is 1 and the other components are all 0.*

In particular, the conditional expectation of the iterated Itô integral is a standard Hermite polynomial given by

$$\mathbb{E}[\mathbb{I}_{\mathbf{i}}(t) \mid W(t) = x] = \frac{\sqrt{t}^{\|\mathbf{i}\|}}{n!} H_{\mathbf{c}_{\mathbf{i}}}\left(\frac{x}{\sqrt{t}}\right). \tag{A5}$$

The explicit formulas (A3) and (A5) were first obtained in Lemmas B.2 and B.3 in [36]. Using these two formulas, in [36] it was demonstrated, through the symbolic computation function in *Mathematica*, that the Hermite expansion and the pathwise expansion of [26] have the same formula up to any given order for one- and two-dimensional diffusions. In this paper we further substantiate the equivalence of the expansion formulas between the Hermite and pathwise expansion methods through theoretical proofs, with the help of the quasi-Lamperti transform.

It is worth mentioning that an alternative polynomial expression for (A5) is also provided in Proposition 3 of [27] and Subsection 4.1 of [28]. However, explicit formulas for the conditional expectation of the product of the iterated Itô integral (A3) are new to the literature. Furthermore, our formulas are expressed in terms of Hermite polynomials, which allows us to derive an expression for the coefficients of the pathwise expansion based on Hermite polynomials.

Appendix B. Proofs of Lemma 1 and Theorem 1

Proof of Lemma 1. For notational simplification, we prove the lemma for the one-dimensional case. The proof for the multidimensional case is as straightforward as in the one-dimensional case.

Recalling the diffusion $Y^\epsilon(s)$, we have

$$\begin{aligned} Y^\epsilon(1) - y &= \epsilon \int_0^1 \sigma^Y(Y^\epsilon(t_1))\,\mathrm{d}W(t_1) + \epsilon^2 \int_0^1 \mu^Y(Y^\epsilon(t_1))\,\mathrm{d}t_1 \\ &= \epsilon \int_0^1 \sigma^Y(y)\,\mathrm{d}W(t_1) + \epsilon \int_0^1 \big(\sigma^Y(Y^\epsilon(t_1)) - \sigma^Y(y)\big)\,\mathrm{d}W(t_1) \\ &\quad + \epsilon^2 \int_0^1 \mu^Y(y)\,\mathrm{d}t_1 + \epsilon^2 \int_0^1 \big(\mu^Y(Y^\epsilon(t_1)) - \mu^Y(y)\big)\,\mathrm{d}t_1. \end{aligned}$$

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Let

$$F_1^Y = \sigma^Y(y)\int_0^1 \mathrm{d}W(t_1) = \sigma^Y(y)\mathbb{I}_{(1)}(1),$$
$$F_2^Y = \mu^Y(y)\int_0^1 \mathrm{d}t_1 + \mathcal{L}_1\sigma^Y(y)\int_0^1\int_0^{t_1} \mathrm{d}W(t_2)\,\mathrm{d}W(t_1) = \mu^Y(y)\mathbb{I}_{(0)}(1) + \mathcal{L}_1\sigma^Y(y)\mathbb{I}_{(1,1)}(1).$$

Applying Itô's formula to the integrands $\sigma^Y(Y^\epsilon(t_1))$ and $\mu^Y(Y^\epsilon(t_1))$, we have

$$\begin{aligned} Y^\epsilon(1) - y = {} & \epsilon F_1^Y + \epsilon^2 F_2^Y \\ & + \epsilon^2\int_0^1\int_0^{t_1} \left(\mathcal{L}_1\sigma^Y(Y^\epsilon(t_2)) - \mathcal{L}_1\sigma^Y(y)\right)\mathrm{d}W(t_2)\,\mathrm{d}W(t_1) \\ & + \epsilon^3\int_0^1\int_0^{t_1} \mathcal{L}_0\sigma^Y(Y^\epsilon(t_2))\,\mathrm{d}t_2\,\mathrm{d}W(t_1) + \epsilon^3\int_0^1\int_0^{t_1} \mathcal{L}_1\mu^Y(Y^\epsilon(t_2))\,\mathrm{d}W(t_2)\,\mathrm{d}t_1 \\ & + \epsilon^4\int_0^1\int_0^{t_1} \mathcal{L}_0\mu^Y(Y^\epsilon(t_2))\,\mathrm{d}t_2\,\mathrm{d}t_1. \end{aligned}$$

The lemma is proved by repeatedly applying Itô's formula to the stochastic integrands and collecting terms according to the order of ϵ. Specifically, the third and fourth expansion coefficients are given here for reference:

$$\begin{aligned} F_3^Y &= \mathcal{L}_0\sigma^Y(y)\int_0^1\int_0^{t_1} \mathrm{d}t_2\,\mathrm{d}W(t_1) + \mathcal{L}_1\mu^Y(y)\int_0^1\int_0^{t_1} \mathrm{d}W(t_2)\,\mathrm{d}t_1 \\ &\quad + \mathcal{L}_1\circ\mathcal{L}_1\sigma^Y(y)\int_0^1\int_0^{t_1}\int_0^{t_2} \mathrm{d}W(t_3)\,\mathrm{d}W(t_2)\,\mathrm{d}W(t_1) \\ &= \mathcal{L}_0\sigma^Y(y)\mathbb{I}_{(1,0)}(1) + \mathcal{L}_1\mu^Y(y)\mathbb{I}_{(0,1)}(1) + \mathcal{L}_1\circ\mathcal{L}_1\sigma^Y(y)\mathbb{I}_{(1,1,1)}(1), \\ F_4^Y &= \mathcal{L}_0\mu^Y(y)\mathbb{I}_{(0,0)}(1) + \mathcal{L}_0\circ\mathcal{L}_1\sigma^Y(y)\mathbb{I}_{(1,1,0)}(1) + \mathcal{L}_1\circ\mathcal{L}_1\mu^Y(y)\mathbb{I}_{(0,1,1)}(1) \\ &\quad + \mathcal{L}_1\circ\mathcal{L}_0\sigma^Y(y)\mathbb{I}_{(1,0,1)}(1) + \mathcal{L}_1\circ\mathcal{L}_1\circ\mathcal{L}_1\sigma^Y(y)\mathbb{I}_{(1,1,1,1)}(1). \end{aligned}$$

This completes the proof of Lemma 1. □

Proof of Theorem 1. Recalling the coefficient $\Omega_k\big(y;f(\cdot)\big)$ in (26), note that we have

$$\Omega_k\big(y;f(\cdot)\big) = \mathbb{E}\big[\Phi_k\big(y;f(\cdot)\big)\big],$$

where $\Phi_k\big(y;f(\cdot)\big)$ is the kth-order pathwise expansion coefficient of $f\big(\sum_{j=0}^K F_{j+1}^Y\epsilon^i + \mathcal{O}(\epsilon^{K+1})\big)$ with respect to ϵ, that is,

$$\Phi_k\big(y;f(\cdot)\big) = \frac{1}{k!}\frac{\mathrm{d}^k}{\mathrm{d}\epsilon^k}\left[f\left(\sum_{j=0}^K F_{j+1}^Y\epsilon^i + \mathcal{O}\left(\epsilon^{K+1}\right)\right)\right]\Big|_{\epsilon=0}.$$

Using the chain rule for kth-order derivatives of the composite function, $\Phi_k\big(y;f(\cdot)\big)$ can be explicitly expressed in terms of the partial derivatives of $f(\cdot)$ and the product of $F_{j+1,i}^Y$ for $1\le j\le k$ and $1\le i\le m$:

$$\Phi_k\big(y;f(\cdot)\big) = \sum_{l=1}^k \frac{1}{l!}\sum_{\mathbf{j}=(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k^l}\ \sum_{\mathbf{r}\in\{1,2,\ldots,m\}^l} \partial_z^{\mathbf{b_r}} f(z)\big|_{z=W(1)}\prod_{\omega=1}^l F_{j_\omega+1,r_\omega}^Y, \tag{B1}$$

where $\mathbf{r} = (r_1,\ldots,r_l)\in\{1,2,\ldots,m\}^l$ and $\mathbf{b_r} = \sum_{\omega=1}^l e_{r_\omega}$.

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To compute the expectation $\Omega_k(y;f(\cdot))=\mathbb{E}[\Phi_k(y;f(\cdot))]$, using the integration by parts formula, we obtain

$$\begin{aligned}\mathbb{E}\left[\partial_z^{\mathbf{b_r}} f(z)\big|_{z=W(1)}\prod_{\omega=1}^{l}F^Y_{j_\omega+1,r_\omega}\right]&=\int_{\mathbb{R}^m}\partial_z^{\mathbf{b_r}}f(z)\left(\mathbb{E}\left[\prod_{\omega=1}^{l}F^Y_{j_\omega+1,r_\omega}\,\middle|\,W(1)=z\right]\phi(z)\right)\mathrm{d}z\\&=(-1)^l\int_{\mathbb{R}^m}f(z)\partial_z^{\mathbf{b_r}}\left(\mathbb{E}\left[\prod_{\omega=1}^{l}F^Y_{j_\omega+1,r_\omega}\,\middle|\,W(1)=z\right]\phi(z)\right)\mathrm{d}z,\end{aligned}\tag{B2}$$

where we have used the fact that $|\mathbf{b_r}|=l$. The conditional expectation is given by

$$\mathbb{E}\left[\prod_{\omega=1}^{l}F^Y_{j_\omega+1,r_\omega}\,\middle|\,W(1)=z\right]=\sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1}\\ \omega=1,\dots,l}}\left(A(y;\ddot{\mathbf{i}},\mathbf{r})\cdot\mathbb{E}\left[\prod_{\omega=1}^{l}\mathbb{I}_{\mathbf{i}_\omega}(1)\,\middle|\,W(1)=z\right]\right),\tag{B3}$$

where $\ddot{\mathbf{i}}=\mathbf{i}_1\wedge\cdots\wedge\mathbf{i}_l$, $A(y;\ddot{\mathbf{i}},\mathbf{r})$ is given by (29), and $\mathcal{M}_j$ is recursively defined by (24). By Lemma 2,

$$\mathbb{E}\left[\prod_{\omega=1}^{l}\mathbb{I}_{\mathbf{i}_\omega}(1)\,\middle|\,W(1)=z\right]=\sum_{0\le\mathbf{a}\le\lfloor\mathbf{c}_{\ddot{\mathbf{i}}}/2\rfloor}\frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}})-|\mathbf{a}|)!}H_{\mathbf{c}_{\ddot{\mathbf{i}}}-2\mathbf{a}}(z).\tag{B4}$$

Furthermore, using the definition of Hermite polynomials and noting that $|\mathbf{b_r}|=l$, we have

$$(-1)^l\partial_z^{\mathbf{b_r}}\left(H_{\mathbf{c}_{\ddot{\mathbf{i}}}-2\mathbf{a}}(z)\phi(z)\right)=(-1)^{l+|\mathbf{c}_{\ddot{\mathbf{i}}}-2\mathbf{a}|}\partial_z^{\mathbf{b_r}+\mathbf{c}_{\ddot{\mathbf{i}}}-2\mathbf{a}}\phi(z)=H_{\mathbf{c}_{\ddot{\mathbf{i}}}-2\mathbf{a}+\mathbf{b_r}}(z)\phi(z).\tag{B5}$$

Plugging (B3), (B4), and (B5) into (B2), we have

$$\begin{aligned}&\mathbb{E}\left[\partial_z^{\mathbf{b_r}}H_h(z)\big|_{z=W(1)}\prod_{\omega=1}^{l}F^Y_{j_\omega+1,r_\omega}\right]\\&\quad=\sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1}\\ \omega=1,\dots,l}}A(y;\ddot{\mathbf{i}},\mathbf{r})\sum_{0\le\mathbf{a}\le\lfloor\mathbf{c}_{\ddot{\mathbf{i}}}/2\rfloor}\frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}})-|\mathbf{a}|)!}\cdot I(f(\cdot),\mathbf{c}_{\ddot{\mathbf{i}}}-2\mathbf{a}+\mathbf{b_r}),\end{aligned}$$

where $I(f(\cdot),\mathbf{h})$ is defined in (27).

Then, the theorem is proved by substituting the above equation into the expectation of (B1); we have $B(f(\cdot);\ddot{\mathbf{i}},\mathbf{r})$ in (33), i.e.

$$B(f(\cdot);\ddot{\mathbf{i}},\mathbf{r})=\sum_{0\le\mathbf{a}\le\lfloor\mathbf{c}_{\ddot{\mathbf{i}}}/2\rfloor}\frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}})-|\mathbf{a}|)!}\cdot I\big(f(\cdot),\mathbf{c}_{\ddot{\mathbf{i}}}-2\mathbf{a}+\mathbf{b_r}\big),$$

where $\ddot{\mathbf{i}}=\mathbf{i}_1\wedge\cdots\wedge\mathbf{i}_l$, $\mathbf{r}=(r_1,\dots,r_l)$, and $\mathbf{b_r}=\sum_{\omega=1}^{l}e_{r_\omega}$, with the remaining details thoroughly explained in Lemma 2. □

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Appendix C. The equivalence of density expansions

C.1. Connection to [26]

For ease of comparison, we explicitly present the density expansion derived in this paper in the following proposition.

Proposition 1. *Given $t' > t$, the transition density function from $X(t) = x$ to $X(t') = x'$ for the diffusion X in (1) has the following expansion:*

$$p_X(t', x' \mid t, x) = \Delta^{-\frac{m}{2}} \det(L) \left(\phi(\gamma) + \sum_{k=1}^{K} \Omega_k\big(y; \delta(\cdot - \gamma)\big) \Delta^{\frac{k}{2}} \right) + \mathcal{O}\big(\Delta^{\frac{K+1-m}{2}}\big), \tag{C1}$$

where $\Delta = t' - t$, $y = Lx$, $y' = Lx'$, $\gamma = (y' - y)/\sqrt{\Delta}$, $\phi(\gamma)$ is the m-dimensional standard normal density function, and the expansion coefficient $\Omega_k\big(y; \delta(\cdot - \gamma)\big)$ is explicitly given by

$$\Omega_k(y; \delta(\cdot - \gamma)) = \phi(\gamma) \sum_{l=1}^{k} \frac{1}{l!} \sum_{\mathbf{j}=(j_1, j_2, \ldots, j_l) \in \mathcal{S}_k^l} \sum_{\mathbf{r} \in \{1,2,\ldots,m\}^l} \sum_{\substack{\mathbf{i}_\omega \in \mathcal{M}_{j_\omega + 1} \\ \omega = 1, \ldots, l}} \left(\prod_{\omega=1}^{l} C^Y_{\mathbf{i}_\omega, r_\omega}(y) \right)$$
$$\cdot \sum_{0 \le \mathbf{a} \le \lfloor \mathbf{c}_{\ddot{\mathbf{i}}}/2 \rfloor} \frac{\tilde{w}_{\mathbf{a}, \ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}}) - |\mathbf{a}|)!} H_{\mathbf{c}_{\ddot{\mathbf{i}}} - 2\mathbf{a} + \mathbf{b}_{\mathbf{r}}}(\gamma). \tag{C2}$$

Here, $\ddot{\mathbf{i}} = \mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l$, $\mathbf{r} = (r_1, \ldots, r_l)$, $\mathbf{b}_{\mathbf{r}} = \sum_{\omega=1}^{l} e_{r_\omega}$, $H_h(\gamma)$ denotes its corresponding multivariate Hermite polynomial, and $\mathcal{S}_k^l$, $\mathcal{M}_j$, $C^Y_{\mathbf{i}_\omega, r_\omega}(y)$, and $\tilde{w}_{\mathbf{a}, \ddot{\mathbf{i}}}$ are recursively defined by (28), (24), (25), and (A4), respectively.

In the following lemma, we show that the density expansion (C1) provides an alternative explicit expression for the expansion formula in [26] and [28]. However, unlike the formula presented in those works, the newly derived formula is explicitly expressed as a linear combination of Hermite polynomials. This form allows us to connect it to the Hermite expansion of [34] and [36].

Lemma 3. *Denote the first term on the right-hand side of (C1) by $p_X^{(K,LI)}(t', x' \mid t, x)$ and the Kth-order expansion provided by (3.21) and (3.25) of [26] by $\tilde{p}_X^{(K,LI)}(t', x' \mid t, x)$. Then these two expansions are the same, that is,*

$$p_X^{(K,LI)}(t', x' \mid t, x) = \tilde{p}_X^{(K,LI)}(t', x' \mid t, x). \tag{C3}$$

Proof of Lemma 3. Using (21) and (44), the quasi-Lamperti transform (16), and the Jacobian formula for the change of variable, we obtain the transition density of X as

$$p_X(t', x' \mid t, x) = \Delta^{-\frac{m}{2}} \det(v_0)^{-1/2} \mathbb{E}\big[\delta(\Gamma^\epsilon - \gamma) \,\big|\, Y(t) = y\big], \tag{C4}$$

where $\Gamma^\epsilon = (Y^\epsilon(1) - y)/\epsilon = (Y(t') - y)/\epsilon$, $\gamma = (y' - y)/\epsilon$, $\epsilon = \sqrt{\Delta}$, and $\Delta = t' - t$.

The expansion $p_X^{(K,LI)}(t', x' \mid t, x)$ of the first term on the right-hand side of (C1) is the Lth-order Taylor expansion of the right-hand side of (C4) with respect to ϵ.

On the other hand, in [26] the transition density of X is characterized as

$$p_X(t', y' \mid t, y) = \Delta^{-\frac{m}{2}} \det(D(x)) \, \mathbb{E}[\delta(\widetilde{Y}^\epsilon - \widetilde{y}) \mid X(t) = x], \tag{C5}$$

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where $D(x)$ is a diagonal matrix given by (3.12) in [26],

$$D(x) = \operatorname{diag}\left\{ \frac{1}{\sqrt{\sum_{j=1}^m \sigma_{1j}^2(x)}}, \ldots, \frac{1}{\sqrt{\sum_{j=1}^m \sigma_{mj}^2(x)}} \right\},$$

$\widetilde{Y}^\epsilon = D(x)(X^\epsilon(1) - x)/\epsilon$, and $\widetilde{y} = D(x)(x' - x)/\epsilon$. The expansion $\tilde{p}_X^{(L,LI)}$ provided by (3.21) and (3.25) of [26] is the Lth-order Taylor expansion of the right-hand side of (C5) with respect to ϵ.

Noting that

$$\widetilde{Y}^\epsilon - \widetilde{y} = D(x)\frac{X^\epsilon(1) - x'}{\epsilon} = D(x)\nu_0^{1/2}(\Gamma^\epsilon - \gamma)$$

by the Jacobian formula for the change of variable, the right-hand sides of (C4) and (C5) are identical. Thus, the lemma is proved. □

C.2. Connection to [34] and [36]

C.2.1. *Recalculating formulas for the Hermite expansion of* [34, 36] *via the pathwise expansion method.* In [34] the transition density of the multivariate diffusion is expanded using Hermite polynomials, with the expansion coefficients being conditional expectations of Hermite polynomials. Further, analytical approximations to these coefficients were obtained through an Itô–Taylor expansion. In this subsection, we use the pathwise expansion method from Theorem 1 to rederive these expansion coefficients. Specifically, by taking f to be a Hermite polynomial, we obtain an alternative analytical approximation for the expansion coefficients. Below we elaborate on this process in detail.

First, we use the Jacobian formula for the change of density:

$$p_X(t', x' \mid t, x) = \det(L) p_Y(t', y' \mid t, y), \tag{C6}$$

where $y = Lx$ and $y' = Lx'$. Then, as in [34], we expand the transition density $p_Y(t', y' \mid t, y)$ about $\phi(\gamma)$ to obtain

$$p_Y^{(J)}(t', y' \mid t, y) = \Delta^{-\frac{m}{2}}\phi(\gamma) + \Delta^{-\frac{m}{2}}\phi(\gamma)\sum_{j=1}^{J}\sum_{|h|=j}\eta^{(h)}(\Delta \mid t, y)\cdot H_h(\gamma), \tag{C7}$$

where $\Delta = t' - t$, $\gamma = (y' - y)/\sqrt{\Delta}$, and the coefficients $\{\eta^{(h)}, h = (h_1, h_2, \ldots, h_m) \in \mathbb{Z}_+^m\}$ are given by the conditional expectations

$$\eta^{(h)}(\Delta \mid t, y) = \frac{1}{h!}\mathbb{E}\left[H_h\left(\frac{Y(t+\Delta) - y}{\sqrt{\Delta}}\right) \middle| Y(t) = y \right]. \tag{C8}$$

Next, we recalculate the Hermite expansion coefficient $\eta^{(h)}$ of (C8) in $p_Y^{(3K)}$ of (C7) using the pathwise expansion method up to the same order $\mathcal{O}(\Delta^{K/2})$. This allows us to derive an alternative expression for the reduced Hermite expansion of [34].

Recalling the conditional expectation defined in (22) and the Hermite expansion coefficient $\eta^{(h)}$ given by (C8), and taking

$$f(\cdot) = H_h(\cdot), \tag{C9}$$

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we can use the formulas obtained in Section 3 to derive alternative approximate formulas for the Hermite expansion coefficients. Specifically, by the orthogonality of the Hermite polynomials, the multivariate integrals in (31) and (32) are now given by

$$\Omega_0\big(y; H_h(\cdot)\big) = \int_{\mathbb{R}^m} H_h(z)\phi(z)\,\mathrm{d}z = \mathbf{1}_{\{h=0\}} \tag{C10}$$

and

$$\int_{\mathbb{R}^m} H_h(z) H_{\mathbf{c_i}-2\mathbf{a}+\mathbf{b_r}}(z)\phi(z)\,\mathrm{d}z = h!\cdot \mathbf{1}_{\{\mathbf{c_i}-2\mathbf{a}+\mathbf{b_r}=h\}}. \tag{C11}$$

Thus, by (26), for $h=(h_1,h_2,\ldots,h_m)\in\mathbb{Z}_+^m$, the coefficients $\eta^{(h)}$ in (C8) can be expanded as

$$\begin{aligned}\eta^{(h)}(\Delta \mid t,y) &= \frac{1}{h!}\Omega_0\big(y; H_h(\cdot)\big) + \frac{1}{h!}\sum_{k=1}^{k}\Omega_k\big(y; H_h(\cdot)\big)\epsilon^k + \mathcal{O}\Big(\Delta^{\frac{K+1}{2}}\Big)\\ &= \frac{1}{h!}\sum_{k=1}^{K}\Omega_k\big(y; H_h(\cdot)\big)\Delta^{\frac{k}{2}} + \mathcal{O}\Big(\Delta^{\frac{K+1}{2}}\Big),\end{aligned} \tag{C12}$$

where the expansion coefficient $\Omega_k(y; H_h(\cdot))$ is explicitly given in (C14) below.

Truncating the coefficient $\eta^{(h)}$ in (C12) at order $\Delta^{\frac{K}{2}}$, plugging it into (C7) for $J=3K$, and using the formula (C14) for $\Omega_k\big(y; H_h(\cdot)\big)$, we get an alternative expression for the Kth-order reduced Hermite expansion of [34]. The result is summarized in the following proposition.

Proposition 2. *Given $t'>t$, the transition density function from $X(t)=x$ to $X(t')=x'$ for the diffusion X in (1) can also be expanded as*

$$\begin{aligned}p_X(t',x' \mid t,x) = \Delta^{-\frac{m}{2}}\det(L)\Bigg(\phi(\gamma) + \phi(\gamma)\sum_{j=1}^{3K}\sum_{|h|=j}\frac{1}{h!}\sum_{k=1}^{K}\Omega_k\big(y; H_h(\cdot)\big)\Delta^{\frac{k}{2}}\cdot H_h(\gamma)\Bigg)\\ + \mathcal{O}\big(\Delta^{\frac{K+1-m}{2}}\big),\end{aligned} \tag{C13}$$

where $\Delta = t'-t$, $y=Lx$, $y'=Lx'$, $\gamma=(y'-y)/\sqrt{\Delta}$, $\phi(\gamma)$ is the m-dimensional standard normal density function, and, for $h=(h_1,h_2,\ldots,h_m)\in\mathbb{Z}_+^m$, the expansion coefficient $\Omega_k\big(y; H_h(\cdot)\big)$ is explicitly given by

$$\begin{aligned}\Omega_k(y; H_h(\cdot)) = \sum_{l=1}^{k}\frac{1}{l!}\sum_{\mathbf{j}=(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k^l}\sum_{\mathbf{r}\in\{1,2,\ldots,m\}^l}\sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1}\\ \omega=1,\ldots,l}}\Bigg(\prod_{\omega=1}^{l}C^Y_{\mathbf{i}_\omega,r_\omega}(y)\Bigg)\\ \cdot\frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}})-|\mathbf{a}|)!}\cdot h!\cdot\mathbf{1}\Big\{\mathbf{a}=\tfrac{\mathbf{c_i}+\mathbf{b_r}-h}{2},\,\mathbf{a}\in\mathbb{Z}^m\Big\},\end{aligned} \tag{C14}$$

where $\ddot{\mathbf{i}}=\mathbf{i}_1\wedge\cdots\wedge\mathbf{i}_l$, $\mathbf{r}=(r_1,\ldots,r_l)$, $\mathbf{b_r}=\sum_{\omega=1}^{l}e_{r_\omega}$, and $\mathcal{S}_k^l$, $\mathcal{M}_j$, $C^Y_{\mathbf{i}_\omega,r_\omega}(y)$, and $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$ are recursively defined by (28), (24), (25), and (A4), respectively.

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C.2.2. *Connection to the Hermite expansion of* [34, 36]. Through direct technical verification, the following lemma shows that the first terms on the right-hand sides of (C1) and (C13) are equal.

Lemma 4. *Denote the first terms on the right-hand sides of* (C1) *and* (C13) *by* $p_X^{(K,LI)}(t', x' \mid t, x)$ *and* $p_X^{(K,WY)}(t', x' \mid t, x)$, *respectively. Then these two terms are equal, that is,*

$$p_X^{(K,LI)}(t', x' \mid t, x) = p_X^{(K,WY)}(t', x' \mid t, x). \tag{C15}$$

Note that the right-hand side of (C15) is an alternative formula for the Hermite expansion (32) in [34], and by Proposition 3 the left-hand side of (C15) is identical to the density expansion (3.21) and (3.25) in [26]. Thus, equation (C15) establishes the equivalence between the pathwise expansion of [26] and the Hermite expansion of [34].

Furthermore, in [34] it is proved that their Hermite expansion is the same as the delta expansion of [36] under the choice of $\mu_0 = 0$. In conclusion, Theorem 2 summarizes the equivalence result.

Proof of Lemma 4. Referring to the first terms on the right-hand sides of (C1) and (C13), write

$$p_Y^{(L,LI)}(t', y' \mid t, y) = \Delta^{-\frac{m}{2}}\phi(\gamma) + \Delta^{-\frac{m}{2}} \sum_{k=1}^{L} \Delta^{\frac{k}{2}} \Omega_k\big(y; \delta(\cdot - \gamma)\big), \tag{C16}$$

where the expansion coefficient $\Omega_k\big(y; \delta(\cdot - \gamma)\big)$ is given by (C2), and

$$p_Y^{(L,WY)}(t', y' \mid t, y) = \Delta^{-\frac{m}{2}}\phi(\gamma) + \Delta^{-\frac{m}{2}}\phi(\gamma) \sum_{j=1}^{3L} \sum_{|h|=j} \frac{1}{h!} \sum_{k=1}^{L} \Omega_k\big(y; H_h(\cdot)\big) \Delta^{\frac{k}{2}} \cdot H_h(\gamma), \tag{C17}$$

where the expansion coefficient $\Omega_k\big(y; H_h(\cdot)\big)$ is given by (C14).

To prove (C15), it is sufficient to show that

$$p_Y^{(K,LI)}(t', y' \mid t, y) = p_Y^{(K,WY)}(t', y' \mid t, y). \tag{C18}$$

In the following we prove (C18).

As the reduced Hermite expansion $p_Y^{(L,WY)}(t', y' \mid t, y)$ given by (C17) and (C14) is arranged according to increasing order of the Hermite polynomials, to compare with it, we first show that the pathwise expansion $p_Y^{(L,LI)}(t', y' \mid t, y)$ given by (C16) and (C2) can also be rearranged according to increasing order of the Hermite polynomials as follows:

$$p_Y^{(L,LI)}(t', y' \mid t, y) = \Delta^{-\frac{m}{2}}\phi(\gamma) + \Delta^{-\frac{m}{2}}\phi(\gamma) \sum_{j=1}^{3L} \sum_{|h|=j} \eta^{(h,LI)}(\Delta \mid t, y) \cdot H_h(\gamma), \tag{C19}$$

where the coefficient $\eta^{(h,LI)}(\Delta \mid t, y)$ is given by

$$\eta^{(h,LI)}(\Delta \mid t, y) = \sum_{k=1}^{L} \Delta^{\frac{k}{2}} \sum_{l=1}^{k} \frac{1}{l!} \sum_{\mathbf{j}=(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k^l} \sum_{\mathbf{r}\in\{1,2,\ldots,m\}^l} \sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1} \\ \omega=1,\ldots,l}} \left(\prod_{\omega=1}^{l} C^Y_{\mathbf{i}_\omega, r_\omega}(y)\right)$$
$$\cdot \frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}}) - |\mathbf{a}|)!} \cdot \mathbf{1}_{\left\{\mathbf{a}=\frac{\mathbf{c}_\mathbf{i}+\mathbf{b}_\mathbf{r}-h}{2}, \mathbf{a}\in\mathbb{Z}^m\right\}}. \tag{C20}$$

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Here, $\ddot{\mathbf{i}} = \mathbf{i}_1 \wedge \cdots \wedge \mathbf{i}_l$, $\mathbf{r} = (r_1, \ldots, r_l)$, $\mathbf{b}_\mathbf{r} = \sum_{\omega=1}^{l} e_{r_\omega}$, $\phi(\gamma)$ and $H_h(\gamma)$ are the m-dimensional standard normal density function and the corresponding multivariate Hermite polynomial, respectively, and $\mathcal{S}_k^l$, $\mathcal{M}_j$, $C^Y_{\mathbf{i}_\omega, r_\omega}(y)$, and $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$ are recursively defined by (28), (24), (25), and (A4), respectively.

If (C19) with (C20) holds, comparing the formulas for $\Omega_k(y; H_h(\cdot))$ in (C14) and $\eta^{(h,LI)}(\Delta \mid t, y)$ in (C20), we have

$$\eta^{(h,LI)}(\Delta \mid t, y) = \frac{1}{h!} \sum_{k=1}^{L} \Omega_k(y; H_h(\cdot)) \Delta^{\frac{k}{2}}. \tag{C21}$$

Upon plugging (C21) into (C19) and comparing the result with (C17), the lemma is proved.

Now we proceed to prove (C19) with (C20). According to the definition of the coefficient $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$ in Lemma 2, $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}} = 0$ if $\min(\mathbf{a}) < 0$ or $\max(2\mathbf{a} - \mathbf{c}_{\ddot{\mathbf{i}}}) > 0$. Thus, we can take the summation in $\mathbf{a}$ over all m-dimensional integers in (C2). Plugging this into (C16), we have

$$p_Y^{(L,LI)}(t', y' \mid t, y) = \Delta^{-\frac{m}{2}} \phi(\gamma) + \Delta^{-\frac{m}{2}} \phi(\gamma) \sum_{k=1}^{L} \Delta^{\frac{k}{2}} \sum_{l=1}^{k} \frac{1}{l!} \sum_{\mathbf{j}=(j_1, j_2, \ldots, j_l) \in \mathcal{S}_k^l} \sum_{\mathbf{r} \in \{1,2,\ldots,m\}^l} \sum_{\substack{\mathbf{i}_\omega \in \mathcal{M}_{j_\omega+1} \\ \omega=1,\ldots,l}}$$
$$\cdot \left(\prod_{\omega=1}^{l} C^Y_{\mathbf{i}_\omega, r_\omega}(y) \right) \sum_{\mathbf{a} \in \mathbb{Z}^m} \tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}} \cdot \frac{1}{(\ell(\ddot{\mathbf{i}}) - |\mathbf{a}|)!} H_{\mathbf{c}_{\ddot{\mathbf{i}}} - 2\mathbf{a} + \mathbf{b}_\mathbf{r}}(\gamma). \tag{C22}$$

Consider the change of variable

$$h = \mathbf{c}_{\ddot{\mathbf{i}}} - 2\mathbf{a} + \mathbf{b}_\mathbf{r}. \tag{C23}$$

Note that in (C23) each component of $\mathbf{c}_{\ddot{\mathbf{i}}} + \mathbf{b}_\mathbf{r} - h$ is even, or $\mathbf{a} = (\mathbf{c}_{\ddot{\mathbf{i}}} + \mathbf{b}_\mathbf{r} - h)/2$ is an integer-valued vector, i.e. $\mathbf{a} \in \mathbb{Z}^m$. Thus, (C22) becomes (for simplification, below we still use both h and $\mathbf{a}$ satisfying the relationship (C23))

$$p_Y^{(L,LI)}(t', y' \mid t, y) = \Delta^{-\frac{m}{2}} \phi(\gamma) + \Delta^{-\frac{m}{2}} \phi(\gamma) \sum_{k=1}^{L} \Delta^{\frac{k}{2}} \sum_{l=1}^{k} \frac{1}{l!} \sum_{\mathbf{j}=(j_1, j_2, \ldots, j_l) \in \mathcal{S}_k^l} \sum_{\mathbf{r} \in \{1,2,\ldots,m\}^l} \sum_{\substack{\mathbf{i}_\omega \in \mathcal{M}_{j_\omega+1} \\ \omega=1,\ldots,l}}$$
$$\cdot \left(\prod_{\omega=1}^{l} C^Y_{\mathbf{i}_\omega, r_\omega}(y) \right) \sum_{h \in \mathbb{Z}^m} \tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}} \cdot \frac{1}{(\ell(\ddot{\mathbf{i}}) - |\mathbf{a}|)!} H_h(\gamma) \cdot \mathbf{1}_{\{h = \mathbf{c}_{\ddot{\mathbf{i}}} - 2\mathbf{a} + \mathbf{b}_\mathbf{r}, \mathbf{a} \in \mathbb{Z}^m\}}. \tag{C24}$$

Interchanging the summations with respect to k and h leads to (see (C20) for the definition of $\eta^{(h,LI)}$)

$$p_Y^{(L,LI)}(t', y' \mid t, y) = \Delta^{-\frac{m}{2}} \phi(\gamma) + \Delta^{-\frac{m}{2}} \phi(\gamma) \sum_{h \in \mathbb{Z}^m} H_h(\gamma) \eta^{(h,LI)}(\Delta \mid t, y). \tag{C25}$$

Then we get (C19) by recalling the definition of $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$. Indeed, to get a nonzero $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$ requires that

$$0 \le 2\mathbf{a} \equiv \mathbf{c}_{\ddot{\mathbf{i}}} + \mathbf{b}_\mathbf{r} - h \le \mathbf{c}_{\ddot{\mathbf{i}}} \iff \mathbf{b}_\mathbf{r} \le h \le \mathbf{c}_{\ddot{\mathbf{i}}} + \mathbf{b}_\mathbf{r}. \tag{C26}$$

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For $\ddot{\mathbf{i}} = \{\mathbf{i}_1, \ldots, \mathbf{i}_l\}$ and $\mathbf{i}_\omega \in \mathcal{M}_{j_\omega+1}$ $(\omega = 1, \ldots, l)$, noting that $|\mathbf{b_r}| = l$ and recalling the definitions of $\mathcal{M}_{j_\omega+1}$ and $\mathcal{S}_k$, we have

$$\begin{aligned} |\mathbf{c}_{\ddot{\mathbf{i}}}| &= \sum_{\alpha=1}^{m} c_{\ddot{\mathbf{i}}}(\alpha) = \sum_{\omega=1}^{l}\sum_{\alpha=1}^{m} c_{\mathbf{i}_\omega}(\alpha) = \sum_{\omega=1}^{l}\big(\|\mathbf{i}_\omega\| - 2c_{\mathbf{i}_\omega}(0)\big) \\ &= \sum_{\omega=1}^{l}(j_\omega + 1) - 2c_{\ddot{\mathbf{i}}}(0) = k + l - 2c_{\ddot{\mathbf{i}}}(0). \end{aligned} \tag{C27}$$

Furthermore, for $1 \le k \le L$ and $(j_1, j_2, \ldots, j_l) \in \mathcal{S}_k$, we have that $1 \le l \le k \le L$. Then, combining (C26) and (C27), we have

$$1 \le l \le |h| \le (k + l - 2c_{\ddot{\mathbf{i}}}(0)) + l \le k + 2l \le 3k \le 3L.$$

This proves that (C19) with (C20) holds. The proof is finished. □

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