Explicit Pathwise Expansion for Multivariate Diffusions and Its Application to Equivalence of Density Expansions

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Abstract

In this paper, we provide expressions based on Hermite polynomials for the pathwise expansion method introduced by Watanabe (1987), Yoshida (1992b) and Li (2013). Our approach has two key innovations. First, we introduce a quasi-Lamperti transform that unitizes the process' diffusion matrix at the initial time, as it corresponds to a multi-dimensional uncorrelated normal distribution, thus facilitating subsequent analysis. Second, by utilizing explicit expressions for the conditional expectation of the multiplication of iterated Itô integrals, we derive explicit formulas for the conditional expectation of the pathwise expansion of a general function on the transformed diffusion. Applying the newly derived method to the conditional expectation of the Dirac delta function and Hermite polynomial functions, respectively, we obtain alternative expressions for the pathwise based density expansion proposed by Li (2013) and the Hermite polynomials based density expansion introduced in Yang et al. (2019) and Wan and Yang (2021). We show that the formulas obtained from these two expansion methods are essentially the same by rearranging the terms according to the increasing order of Hermite polynomials.

KEYWORD: Pathwise expansion, Hermite expansion, Quasi-Lamperti transform, Equivalence, Multivariate diffusions, Transition densities

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1 Introduction

Multivariate diffusions governed by stochastic differential equations (SDEs) are widely used in financial economics to describe the evolution of the vector of economic variables including prices, stochastic volatilities, interest rates, and other state variables. Transition densities are pivotal for pricing financial derivatives, implementing maximum likelihood estimation method, and testing models based on discrete observations, see, e.g., Aït-Sahalia (2009). However, the transition density is unknown for most multivariate diffusions.

The theory of Watanabe (1987) in Mallavin calculus and its subsequent developments, termed as the pathwise expansion approach, provides a powerful tool for approximating conditional expectations of generalized functions on a given diffusion process, namely Wiener functionals. The pathwise expansion approach has wide-range applications in statistics and option pricing. On one hand, Yoshida (1992a,b) obtains expansions of statistics and establish statistical properties for maximum likelihood estimator. Li (2013) proposes a pathwise expansion of the Dirac delta function on the diffusion to approximate the transition density, where the expansion coefficient calculated recursively through conditional expectations of iterated stochastic integrals. On the other hand, Takahashi (1999), Kunitomo and Takahashi (2001, 2003), and Li (2014) use the pathwise expansion to approximate option prices. For comprehensive overviews, refer to Bompis and Gobet (2013) and Takahashi (2015).

Moreover, alternative methods of density expansions have also held a significant role within the literature. The Kolmogorov method introduced by Aït-Sahalia (2008) postulates a suitable form for the (log-)transition densities. It expands densities in both time and state variables, and then utilizes the Kolmogorov equations to compute expansion coefficients. Yang et al. (2019) proposes a delta expansion method for approximating transition densities, employing the Itô-Taylor expansion of the conditional expectation of the Dirac delta function. By extending Aït-Sahalia (2002)'s Hermite expansion for univariate diffusions, Wan and Yang (2021) establishes a multivariate version and links it with Yang et al. (2019)'s delta expansion method. For other refinements of density expansions and applications, refer to Aït-Sahalia and Yu (2006), Aït-Sahalia and Kimmel (2007, 2010), Filipović et al. (2013), Choi (2013, 2015), among others.

Deriving explicit formulas for coefficients of the pathwise expansion method is a challenging task. Li (2013, 2014) make significant contributions to this topic. However, the building blocks of Li (2013, 2014)' formulas are the conditional expectation of the multiplication of iterated

Stratonovich integrals. Deriving explicit formulas for these conditional expectation is also a challenging task.[1] Furthermore, the relationship between different expansions for transition densities of multivariate diffusions remains unclear.

In this paper, initially, we derive explicit expansion formulas for the pathwise expansion approach, and subsequently, we employ the result to show the equivalence between existing density expansions. The validity of the pathwise expansion method follows Watanabe theory in Malliavin calculus developed by Watanabe (1987), as well as further analysis of Yoshida (1992b) and Li (2013).

To commence, we obtain formulas based on Hermite polynomials for the pathwise expansion method introduced by Watanabe (1987), Yoshida (1992b), and Li (2013). These formulas allow us to compute the conditional expectation of a *"general function"* on the diffusions, facilitating calculations of the transition density, option prices, and moments. To achieve this goal, we first introduce a *quasi-Lamperti transform* that unitizes the process' diffusion matrix at the initial time, enabling subsequent analysis. Then, we apply the theory of Watanabe (1987), Yoshida (1992b) and Li (2013) to establish a pathwise Taylor expansion for a function on the transformed diffusion. By utilizing explicit expressions for the conditional expectation of the multiplication of iterated Itô integrals, we derive explicit expressions for the conditional expectation of the expansion coefficients.

By considering the *"general function"* within the conditional expectation as the Dirac delta function and Hermite polynomial functions, respectively, we derive alternative expressions for the pathwise method based density expansion proposed by Li (2013) and the Hermite method based density expansion introduced in Yang et al. (2019) and Wan and Yang (2021). The new formulas allow us to collect the terms in the density expansion of Li (2013) according to the ascending order of Hermite polynomials. As a consequence, we establish the equivalence between Li (2013)'s pathwise expansion method and the Hermite expansion method introduced by Yang et al. (2019) and Wan and Yang (2021).

This paper contributes to the literature in two aspects. First, we demonstrate that adopting the quasi-Lamperti transform and explicit expressions for the conditional expectation of the

[1] Section 4 of Li et al. (2016) provides a six-page explanation to address this issue. As a comparison, this paper uses the conditional expectation of the multiplication of iterated Itô integrals to avoid the conditional expectation of the multiplication of iterated Stratonovich integrals and provides explicit formulas for them; see Lemma 3.2. Furthermore, these formulas make it possible to establish equivalence with other expansion methods.

multiplication of iterated Itô integrals facilitates the computation of conditional expectation via the pathwaise Taylor expansion method.

In comparison to Li (2013)'s approach, which uses a diagonal matrix transformation leading to a multi-dimensional *correlated* Brownian motion as the leading term, our quasi-Lamperti transform yields an *uncorrelated* multi-dimensional standard Brownian motion. Consequently, we can avoid calculating high-order derivatives for the general multivariate Hermite polynomials, as indicated in (33) of Theorem 3.1, (39) of Theorem 4.1, (49) of Theorem 4.2. This innovation enables us to reorganize terms according to the increasing order of Hermite polynomials.[2] It will have the same advantage when using the pathwise method to expand other conditional expectations, such as the option prices, moments or cumulative distribution functions.

Second, we rigorously establish the equivalence of the density expansions between the pathwise expansion of Li (2013) and the Hermite expansion of Yang et al. (2019) and Wan and Yang (2021). This substantiates that the Hermite expansion presented in Wan and Yang (2021), with its explicit recursive formulas, offers an alternative representation for the density expansion elucidated in Li (2013).

Organization of the paper. The rest of the paper is organized as follows. Section 2 gives the model setting. Section 3.1 introduces the quasi-Lamperti transform which transforms the original multivariate diffusion X into a transformed diffusion Y. Section 3.2 derives expressions based on Hermite polynomials for the conditional expectation of function f on a normalization of Y via the pathwise expansion method. By taking f to be the Dirac delta function and the Hermite polynomials, Section 4.1 and Section 4.2 recalculate the density expansion formula for the pathwise expansion of Li (2013) and the Hermite expansion method of Yang et al. (2019) and Wan and Yang (2021), respectively, and Section 4.3 establishes the equivalence of two methods. Section 5 backtracks the density expansion for the original process X, and develops the equivalence between the pathwise expansion of Li (2013) and the Hermite expansion of Yang et al. (2019) and Wan and Yang (2021). Section 6 concludes the paper. Technical proofs are collected in the Appendix.

[2] We can recursively define Hermite polynomials associated with multivariate *correlated* normal distributions. In this case, when it comes to calculating high-order derivatives of a function combined with Hermite polynomials, a recursive formulation is not achievable. However, in a sharp contrast, the Hermite polynomials associated with multi-dimensional *uncorrelated* normal distributions emerge as straightforward products of their univariate counterparts. Remarkably, these polynomials exhibit explicit expressions for their high-order derivatives.

Notations. For ease of exposition, we will use the following notational conventions throughout the paper. Note that the positive integer m represents the dimension of the state variable. Let $\mathbb{Z}^m$ be the set of m-dimensional integers, and $\mathbb{Z}_+^m$ be the subset of $\mathbb{Z}^m$, the element of which has nonnegative component. For $h = (h_1, h_2, \cdots, h_m) \in \mathbb{Z}_+^m$, define $|h| := \sum_{i=1}^m h_i$ and $h! = h_1! \cdots h_m!$. Let e_i be a special index vector, in which the i-th component is 1, and the others are 0. We write $x^h = x_1^{h_1} \cdots x_m^{h_m}$ for any $x = (x_1, \ldots, x_m)^\top \in \mathbb{R}^m$, 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 i-th element of the vector μ without confusion. Similarly, denote the (i,j)-element of the matrix ν to be ν_{ij} or $(\nu)_{ij}$. Let $\phi(x)$ denote the density of the standard m-dimensional multivariate normal distribution with mean 0 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_i-th order standard univariate Hermite polynomial.

2 The Model

Consider a multivariate time homogeneous diffusion process

$$dX(s) = \mu^X(X(s))dt + \sigma^X(X(s))dW(s), \tag{1}$$

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 d-dimensional standard Brownian motion, $\mu^X(X(s)) \in \mathbb{R}^m$ and $\sigma^X(X(s)) \in \mathbb{R}^{m \times d}$ are an $m \times 1$ drift vector and an $m \times d$ volatility (or dispersion) matrix, respectively. The explicit forms of μ^X and σ^X are known. Given two time points t and t' such that $t' > t$, let $p_X(t', x'|t, x)$ denote the conditional density of $X(t') = x'$ given $X(t) = x$. Without loss of generality, we assume $m = d$. The diffusion matrix is defined below

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

We need the following technical assumptions to proceed the analysis, which are sufficient to ensure the existence and uniqueness of a solution to SDE (1) with appropriate regularities (Karatzas and Shreve, 1991). These assumptions are also standard in the literature of the transition density expansions for diffusion processes (Watanabe, 1987; Yoshida, 1992b; Li, 2013).

Assumption 1. *The diffusion matrix* $\nu^X(x)$ *is positive definite; i.e.* $\zeta^\top \nu^X(x)\zeta > 0$ *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.*

3 Explicit formulas for the pathwise expansion method via Hermite polynomials

In this section, we first introduce a novel *quasi-Lamperti transform* that transforms the original diffusion X into a new one Y whose diffusion matrix is the identity matrix at the initial time.[3] This transformation makes the subsequent analysis possible. Then we derive explicit formulas for the pathwise expansion of the conditional expectation the transformed process.

3.1 Quasi-Lamperti Transform $X \to Y$

For fixed initial time t and state $X(t) = x$, define a process Y by the following linear transformation

$$Y(s) := \nu_0^{-1/2} X(s), \quad s \geq t, \tag{3}$$

where the constant matrix $\nu_0 := \nu^X(x)$ is non-degenerate by Assumption 1. The dynamics of Y defined by (3) satisfies

$$dY(s) = \mu^Y(Y(s))ds + \sigma^Y(Y(s))dW(s), \quad Y(t) = y, \tag{4}$$

where $y = \nu_0^{-1/2}x$, $\zeta = \nu_0^{-1/2}\xi$, $\mu^Y(\zeta) = \nu_0^{-1/2}\mu^X(\xi)$, and $\sigma^Y(\zeta) = \nu_0^{-1/2}\sigma^X(\xi)$. The diffusion matrix of the diffusion Y is given by

$$\nu^Y(\zeta) = \sigma^Y(\zeta)\sigma^Y(\zeta)^\top.$$

Thus at time t, we can verify that the initial diffusion matrix of Y is the identity matrix, i.e.,

$$\nu^Y(y) = \sigma^Y(y)\sigma^Y(y)^\top = \nu_0^{-1/2}\sigma^X(x)\sigma^X(x)^\top \nu_0^{-1/2} = Id_m, \tag{5}$$

[3]For univariate diffusions, the Lamperti transform can unitize the diffusion of the process throughout the whole time domain. For multivariate diffusions, in general the Lamperti transform does not exist. However, as we aim to derive a small time expansion, the *quasi-Lamperti transform* which unitizes the diffusion matrix at the initial time is enough.

where Id_m is the m-dimensional identity matrix. The transformation defined through (3) is said to be a *quasi-Lamperti transform*.[4] The differential operators associated with Y are given below:

$$\mathcal{L}_{\zeta}^{Y,0} = \sum_{k=1}^{m} \mu_k^Y(\zeta)\partial_{\zeta}^{e_k} + \frac{1}{2}\sum_{k,l=1}^{m} \nu_{kj}^Y(\zeta)\partial_{\zeta}^{e_k+e_l}, \tag{6}$$

$$\mathcal{L}_{\zeta}^{Y,l} = \sum_{k=1}^{m} \sigma_{kl}^Y(\zeta)\partial_{\zeta}^{e_k}, \quad l = 1, \ldots, m. \tag{7}$$

Remark 3.1. *Note that $p_X(t', x'|t, x)$ and $p_Y(t', y'|t, y)$ are transition densities for the original process X and the transformed diffusion Y, respectively. By the Jacobian formula for the change of density, we have*

$$p_X(t', x'|t, x) = \det(\nu_0)^{-1/2} p_Y(t', \nu_0^{-1/2}x'|t, \nu_0^{-1/2}x). \tag{8}$$

Thus, once we have derived a L-th order density expansion, denoted as $p_Y^{(L)}(t', y'|t, y)$ for Y, we can backtrack a density expansion, $p_X^{(L)}(t', x'|t, x)$, of the original process X analogy to (8) as follows,

$$p_X^{(L)}(t', x'|t, x) = \det(\nu_0)^{-1/2} p_Y^{(L)}(t', \nu_0^{-1/2}x'|t, \nu_0^{-1/2}x).$$

3.2 Explicit formulas for the pathwise expansion method

In this subsection, we apply the method of Watanabe (1987), Yoshida (1992b) and Li (2013) to given a pathwise expansion of $f\big(\frac{Y(t')-y}{\sqrt{t'-t}}\big)$ for a given "function" f, and then use the newly derived formula for the conditional expectation of the multiplication of iterated Itô integrals to present a Hermite polynomial based expression for the following conditional expectation

$$\mathbb{E}\left[f\left(\frac{Y(t')-y}{\sqrt{t'-t}}\right)\middle|Y(t) = y\right]. \tag{9}$$

The function $f(\cdot)$ can be a generalized function such as the Dirac delta function, an indicator function, a Lipschitz function, etc. Such choice of f has wide applications in the expansion of transition densities and option prices, etc. For these functions, the validity of the pathwise expansion discussed in this paper is ensured by Watanabe theory in Malliavin calculus, see, e.g., Watanabe (1987); Yoshida (1992b); Li (2013, 2014). For ease of exposition, we do not impose explicit conditions on the function $f(\cdot)$.

[4] If the initial volatility matrix $\sigma^X(x)$ of X is invertible, we can use an alternative quasi-Lamperti transform as follows: $Y(s) := \left(\sigma^X(x)\right)^{-1} X(s)$ for $s \geq t$.

Three main steps for deriving explicit expansion coefficients are presented in Sections 3.2.1, 3.2.2, and 3.2.3 below.

3.2.1 Rescaling the process Y

Rescale the process Y defined by (4) as $Y^\epsilon(s) := Y(\epsilon^2 s + t)$, $s \geq 0$, where $\epsilon := \sqrt{\Delta} = \sqrt{t' - t}$. By (4), we have

$$dY^\epsilon(s) = \epsilon^2 \mu^Y(Y^\epsilon(s))ds + \epsilon\sigma^Y(Y^\epsilon(s))dW^\epsilon(s), \quad Y^\epsilon(0) = y, \tag{10}$$

where $\{W^\epsilon(s), s \geq 0\}$ is a m-dimensional standard Brownian motion. For simplicity, we write $W^\epsilon(s)$ as $W(s)$ when there is no confusion.

Note that $\frac{Y(t')-y}{\sqrt{t'-t}} = \frac{Y^\epsilon(1)-y}{\epsilon}$ since $Y^\epsilon(1) = Y(t')$ and $\epsilon = t' - t$. Define a normalization Γ^ϵ of $Y^\epsilon(1)$ as follows:

$$\Gamma^\epsilon := \frac{Y^\epsilon(1) - y}{\epsilon} \to W(1), \text{ as } \epsilon \to 0. \tag{11}$$

The convergence result above holds because $\sigma^Y(y)$ is an identity matrix, cf. (5).

It's worth mentioning that the normalization Γ^ϵ here corresponds to the standardization in Equation (3.16) of Li (2013), but there are significant differences between the two. Li (2013) uses a diagonal matrix transformation to standardize the original diffusion X leading to a multi-dimensional *correlated* Brownian motion (see Equation (3.17) of Li, 2013). Unlike Li (2013), we use the *quasi-Lamperti transform* and the normalization Γ^ϵ here converges to the *uncorrelated* multi-dimensional standard Brownian motion $W(1)$, which facilitates subsequent analysis. This is one of the two key innovations that sets this paper apart from the computation of Li (2013).

With the normalization Γ^ϵ in (11), the conditional expectation (9) now becomes

$$\mathbb{E}\left[f\left(\frac{Y(t') - y}{\sqrt{t' - t}}\right)\Big|Y(t) = y\right] = \mathbb{E}\left[f(\Gamma^\epsilon)\Big|Y^\epsilon(0) = y\right]. \tag{12}$$

3.2.2 Expanding $f(\Gamma^\epsilon)$ with respect to ϵ

According to Theorem 3.3 of Watanabe (1987), we have the pathwise expansion of the random variable $Y^\epsilon(1)$ in Lemma 3.1 via successive application of Itô formula. Before presenting the results, we introduce some notations first. Consider an *index* $\mathbf{i} = (i_1, i_2, \ldots, i_n) \in \{0, 1, \ldots, m\}^n$ associated with the "norm"

$$\|\mathbf{i}\| = \sum_{l=1}^{m}(2 \cdot \mathbf{1}_{\{i_l=0\}} + \mathbf{1}_{\{i_l\neq 0\}}). \tag{13}$$

Define a set of the indices as follows:

$$\mathcal{M}_k = \{\mathbf{i} = (i_1, i_2, \ldots, i_n)\big| \|\mathbf{i}\| = k\}. \tag{14}$$

Note that we can also recursively define $(\mathcal{M}_k)_{k\geq 0}$ below: $\mathcal{M}_0 = \emptyset$, $\mathcal{M}_1 = \{(1), \cdots, (m)\}$, and

$$\mathcal{M}_{k+1} = \{\mathbf{i}\big| i_1 = 0,\ (i_2, \ldots, i_n) \in \mathcal{M}_{k-1}\} \bigcup_{\alpha=1}^{m} \{\mathbf{i}\big| i_1 = \alpha,\ (i_2, \ldots, i_n) \in \mathcal{M}_k\}. \tag{15}$$

The lemma below gives a pathwise expansion of $Y^{\epsilon}(1)$ via the iterated Itô integral, instead of the iterated Stratonovich integral in Lemma 1 of Li (2013).

Lemma 3.1. *The expansion of the random variable $Y^{\epsilon}(1)$ now reads as*

$$Y^{\epsilon}(1) = \sum_{k=0}^{L} \epsilon^k F_k^Y + \mathcal{O}\Big(\epsilon^{L+1}\Big), \tag{16}$$

where $F_0^Y = y$, and the expansion coefficients have the following general form

$$F_k^Y = \sum_{\mathbf{i}\in\mathcal{M}_k} C_{\mathbf{i}}^Y(y) \cdot \mathbb{I}_{\mathbf{i}}(1), \tag{17}$$

where $\mathbf{i} = (i_1, i_2, \ldots, i_n)$, $\mathcal{M}_k$ is given by (14), and

$$C_{\mathbf{i}}^Y(\zeta) = (\mathcal{L}_{\zeta}^{Y,i_n} \circ \cdots \circ \mathcal{L}_{\zeta}^{Y,i_2})\sigma_{\cdot i_1}^Y(\zeta). \tag{18}$$

Here $\sigma_{\cdot 0}^Y = \mu^Y$, $\sigma_{\cdot i_1}^Y = (\sigma_{1i_1}^Y, \cdots, \sigma_{mi_1}^Y)^{\top}$, and the operators are defined by (6)-(7). The iterated Itô integral $\mathbb{I}_{\mathbf{i}}(t)$ is defined through

$$\mathbb{I}_{\mathbf{i}}(t) = \int_0^t \int_0^{t_1} \cdots \int_0^{t_{n-1}} dW_{i_n}(t_n) \cdots dW_{i_2}(t_2) dW_{i_1}(t_1), \tag{19}$$

where $W_0(t) = t$ by convention.

Then the pathwise expansion (16) and the definition in (11) imply that

$$\Gamma^{\epsilon} = \sum_{j=0}^{L} F_{j+1}^Y \epsilon^i + \mathcal{O}(\epsilon^{L+1}). \tag{20}$$

Using the chain rule for differentiating composite functions,[5] we have

$$f(\Gamma^{\epsilon}) = f(W(1)) + \sum_{k=1}^{L} \Phi_k\big(y; f(\cdot)\big)\epsilon^k + \mathcal{O}(\epsilon^{L+1}). \tag{21}$$

[5]See Theorem 3.5 of Watanabe (1987); Theorem 2.2 of Yoshida (1992b); Appendix B.1 of Li (2013) for the cases that f is a generalized function.

The coefficient $\Phi_k\big(y; f(\cdot)\big)$ can be represented explicitly in terms of the derivatives of $f(\cdot)$ and the product of $F_j^Y, 1 \leq j \leq k$, that is,

$$\Phi_k\big(y; f(\cdot)\big) = \sum_{(j_1,j_2,\dots,j_l)\in\mathcal{S}_k} \sum_{\mathbf{r}\in\{1,2,\dots,m\}^l} \frac{1}{l!}\partial_z^{\mathbf{b_r}} f(z)\Big|_{z=W(1)} \prod_{\omega=1}^{l} F^Y_{j_\omega+1,r_\omega}, \tag{22}$$

where $\mathbf{r} := (r_1, \dots, r_l) \in \{1, 2, \dots, m\}^l$, $\mathbf{b_r} := \sum_{\omega=1}^{l} e_{r_\omega}$, $F^Y_{j_\omega+1}$ is given by (17), and $\mathcal{S}_k$ is defined below

$$\mathcal{S}_k = \big\{\mathbf{j} := (j_1, j_2, \dots, j_l)\big| j_\omega \geq 1, \omega = 1, \cdots, l;\ j_1 + j_2 + \cdots + j_l = k;\ l = 1, 2, \dots\big\}. \tag{23}$$

Note that we can also define $(\mathcal{S}_k)_{k\geq1}$ recursively by $\mathcal{S}_1 = \{(1)\}$ and

$$\mathcal{S}_{k+1} = \{\mathbf{j}\ |j_1 = 1,\ (j_2, \dots, j_l) \in \mathcal{S}_k\} \cup \{\mathbf{j}\ |(j_1 - 1, j_2, \dots, j_l) \in \mathcal{S}_k\}. \tag{24}$$

3.2.3 Computing the expansion coefficients

To compute the conditional expectation (9) or (12), i.e., $\mathbb{E}[f(\Gamma^\epsilon)|Y^\epsilon(0) = y]$, we take conditional expectation on both sides of (21), which leads to

$$\mathbb{E}\left[f\left(\frac{Y(t') - y}{\sqrt{t' - t}}\right)\Big|Y(t) = y\right] = \Omega_0\big(y; f(\cdot)\big) + \sum_{k=1}^{L} \Omega_k\big(y; f(\cdot)\big)\epsilon^k + \mathcal{O}(\epsilon^{L+1}), \tag{25}$$

where $\Omega_0\big(y; f(\cdot)\big) = \mathbb{E}[f(W(1))]$ and for $k = 1, \dots, L$

$$\Omega_k\big(y; f(\cdot)\big) := \mathbb{E}[\Phi_k\big(y; f(\cdot)\big)]. \tag{26}$$

The leading order term is

$$\Omega_0\big(y; f(\cdot)\big) = \int_{\mathbb{R}^m} f(z)\,\phi(z)dz. \tag{27}$$

For the k-th order term, noting that $\Phi_k\big(y; f(\cdot)\big)$ is given by (22), the conditional expectation of the multiplication of the iterated Itô integrals, i.e.,

$$\mathbb{E}\left[\prod_{\omega=1}^{l} \mathbb{I}_{\mathbf{i}_\omega}(t)\Big|W(t) = x\right], \tag{28}$$

plays a key role. Lemma 3.2 below gives an explicit recursive formulas for (28). It is worth mentioning that by replacing the iterated Itô integrals in (28) with iterated Stratonovich integrals, the conditional expectation of the multiplication of iterated Stratonovich integrals are the building blocks of the pathwise expansion proposed by Li (2013). Appendix A of Li (2013) provides an effective algorithm with three major steps for computing these conditional expectations, which are further discussed by Section 4 of Li (2014) and Section 4 of Li et al. (2016). Compared to algorithms described on several pages in Li (2013, 2014) and Li et al. (2016), our approach does not involve the Stratonovich integrals and thus we do not need algorithms that convert the multiplication of iterated Stratonovich integrals to the iterated Itô integrals. In addition, our formula in Lemma 3.2 is explicit and easier for readers to implement.

Let $\ddot{\mathbf{i}} := \{\mathbf{i}_1, \cdots, \mathbf{i}_l\}$ be a vector whose components are *indices* of the iterated Itô integrals (19). Define the "norm" $\|\ddot{\mathbf{i}}\| = \sum_{\omega=1}^{l} \|\mathbf{i}_\omega\|$, where $\|\mathbf{i}_\omega\|$ is given by (13). Let $n_{\mathbf{i}_\omega}(\alpha)$ and $n_{\ddot{\mathbf{i}}}(\alpha)$ be the number of α ($\alpha = 0, 1, \cdots, m$) in $\mathbf{i}_\omega$ and $\ddot{\mathbf{i}}$, respectively, that is, $n_{\mathbf{i}_\omega}(\alpha) = \sum_{k=1}^{n} \mathbf{1}_{\{(\mathbf{i}_\omega)_k=\alpha\}}$ and $n_{\ddot{\mathbf{i}}}(\alpha) = \sum_{\omega=1}^{l} n_{\mathbf{i}_\omega}(\alpha)$. We can further define $\mathbf{n}_{\mathbf{i}_\omega} = (n_{\mathbf{i}_\omega}(1), \cdots, n_{\mathbf{i}_\omega}(m))$ and $\mathbf{n}(\ddot{\mathbf{i}}) = \sum_{\omega=1}^{l} \mathbf{n}_{\mathbf{i}_\omega}$. Let $\ell(\ddot{\mathbf{i}})$ be the total length of all *indices* $\mathbf{i}_\omega$ (for $\omega = 1, \ldots, l$) in $\ddot{\mathbf{i}}$, that is,

$$\ell(\ddot{\mathbf{i}}) = n_{\ddot{\mathbf{i}}}(0) + \sum_{\alpha=1}^{m} n_{\ddot{\mathbf{i}}}(\alpha) = \sum_{\omega=1}^{l} \left(n_{\mathbf{i}_\omega}(0) + \sum_{\alpha=1}^{m} n_{\mathbf{i}_\omega}(\alpha) \right). \tag{29}$$

With these notations, we can present the explicit formula for the conditional expectation of the product of iterated Itô integrals in lemma below.

Lemma 3.2. *The conditional expectation of the product of iterated Itô integrals is a linear combination of the Hermite polynomials as follows*

$$\mathbb{E}\left[\prod_{\omega=1}^{l} \mathbb{I}_{\mathbf{i}_\omega}(t) \middle| W(t) = x \right] = \sum_{0 \le \boldsymbol{a} \le \lfloor \mathbf{n}(\ddot{\boldsymbol{i}})/2 \rfloor} \tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{i}}} \cdot \left(\frac{\sqrt{t}^{\|\ddot{\boldsymbol{i}}\|}}{(\ell(\ddot{\boldsymbol{i}}) - |\boldsymbol{a}|)!} H_{\mathbf{n}(\ddot{\boldsymbol{i}})-2\boldsymbol{a}} \left(\frac{x}{\sqrt{t}} \right) \right), \tag{30}$$

where $\ddot{\boldsymbol{i}} := \{\mathbf{i}_1, \cdots, \mathbf{i}_l\}$*,* $\boldsymbol{a} = (a_1, \cdots, a_m)$*. The coefficient* $\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{i}}}$ *is recursively determined as follows:* $\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{i}}} = \mathbf{1}_{\{\boldsymbol{a}=0\}}$ *if* $\ddot{\boldsymbol{i}} = \emptyset$ *or* $\{\mathbf{i}_1\}$*;* $\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{i}}} = 0$ *if* $\min(\boldsymbol{a}) < 0$ *or* $\max(2\boldsymbol{a} - \mathbf{n}(\ddot{\boldsymbol{i}})) > 0$*; and*

$$\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{i}}} = \sum_{\omega_1=1}^{l} \tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{i}}_{-\omega_1}} + \sum_{1 \le \omega_1 < \omega_2 \le l} \mathbf{1}_{\{(i_{\omega_1})_1 = (i_{\omega_2})_1 \neq 0\}} \tilde{w}_{\boldsymbol{a}-e_{(i_{\omega_1})_1}, \ddot{\boldsymbol{i}}_{-\omega_1-\omega_2}}, \tag{31}$$

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

In particular, the conditional expectation of the iterated Itô integral defined in (19) is a standard Hermite polynomial given below:

$$\mathbb{E}[\mathbb{I}_{\mathbf{i}}(t) | W(t) = x] = \frac{\sqrt{t}^{\|\mathbf{i}\|}}{n!} H_{\mathbf{n}_{\mathbf{i}}} \left(\frac{x}{\sqrt{t}} \right). \tag{32}$$

The explicit formulas (30) and (32) are first obtained in Lemmas B.2 and B.3 in Yang et al. (2019). Using these two formulas, Yang et al. (2019) demonstrate that the Hermite expansion and the pathwise expansion of Li (2013) have the same formulas up to any given order for one- and two-dimensional diffusions through the symbolic computation function in *Mathematica*. 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 (32) is also provided by Proposition 3 in Li (2014) and Section 4.1 of Li et al. (2016). However, explicit formulas for the conditional expectation of the product of the iterated Itô integral (30) is new in 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.

In detail, using the explicit formulas (30) and (32) for the conditional expectation of the product of the iterated Itô integral presented in Lemma 3.2, we can derive an explicit recursive formulas for the coefficients $\Omega_k\big(y; f(\cdot)\big)$. These coefficients associated with the pathwise expansion method for the transformed process Y defined (4), with its initial diffusion matrix being the identity matrix. The result is presented in the theorem below.

Theorem 3.1. *The expansion coefficient $\Omega_k\big(y; f(\cdot)\big)$ in (25) is explicitly given by*

$$\Omega_k\big(y; f(\cdot)\big) = \sum_{(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k} \frac{1}{l!} \sum_{\boldsymbol{r}\in\{1,2,\ldots,m\}^l} \sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1}\\ \omega=1,\cdots,l}} \left(\prod_{\omega=1}^{l} C^{Y}_{\mathbf{i}_\omega, r_\omega}(y)\right)$$
$$\cdot \sum_{0\le \boldsymbol{a}\le\lfloor \mathbf{n}(\ddot{\boldsymbol{\imath}})/2\rfloor} \cdot \frac{\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{\imath}}}}{(\ell(\ddot{\boldsymbol{\imath}})-|\boldsymbol{a}|)!} \cdot \int_{\mathbb{R}^m} f\,(z)\, H_{\mathbf{n}(\ddot{\boldsymbol{\imath}})-2\boldsymbol{a}+\boldsymbol{b}_{\boldsymbol{r}}}\,(z)\,\phi(z)dz, \tag{33}$$

where $\boldsymbol{r} := (r_1,\ldots,r_l)$, $\boldsymbol{b}_{\boldsymbol{r}} := \sum_{\omega=1}^{l} e_{r_\omega}$, $\phi(z)$ is the m-dimensional standard normal density function and $H_h(z)$ denotes its corresponding multivariate Hermite polynomial, $\mathcal{S}_k$, $\mathcal{M}_j$, $C^{Y}_{\mathbf{i}_\omega,r_\omega}(y)$ and $\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{\imath}}}$ are recursively defined by (24), (15), (18) and (31), respectively.

To calculate the explicit formulas for the expansion of (9) given by (25), (27) and (33), we need to compute multivariate integrals in (27) and (33). For certain special functions such as the Dirac delta function, the Hermite polynomial, and the option payoff function, these multivariate integrals in (27) and (33) can be simplified into analytical formulas without the need for integration. In the next section, we provide explicit formulas to compute the multivariate integrals in (27) and (33) for the Dirac delta function and the Hermite polynomials, in order to recalculate formulas for the pathwise expansion of Li (2013) and the Hermite expansion of Yang et al. (2019) and Wan and Yang (2021), respectively.

4 Equivalence of density expansions for the transformed process Y

In this section, we focus on the transformed diffusion process Y defined in (4). Specially, we apply the result of Theorem 3.1 to recalculate the density expansion formulas for both the pathwise expansion of Li (2013) and the Hermite expansion of Yang et al. (2019) and Wan and Yang (2021). This allows us to demonstrate their equivalence under the process Y.

4.1 Recalculate formulas for the pathwise expansion of Li (2013)

Li (2013) starts from the fact that the transition density admits the following representation

$$p_Y(t',y'|t,y) = \mathbb{E}[\delta(Y(t')-y')|Y(t)=y], \tag{34}$$

where $\delta(\cdot)$ is the Dirac delta function, see, e.g, Watanabe (1987). We can rewrite it using the Jacobian formula for the change of density as follows:

$$p_Y(t',y'|t,y) = \Delta^{-\frac{m}{2}}\mathbb{E}\left[\delta\left(\frac{Y(t')-y}{\sqrt{\Delta}}-\gamma\right)\Big|Y(t)=y\right], \tag{35}$$

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

Recalling the conditional expectation defined in (9) and the transition density given by (35), and considering

$$f(\cdot) = \delta(\cdot-\gamma), \tag{36}$$

we can provide explicit formulas for Li (2013)' density expansion using the formulas derived in Section 3. Specifically, the multivariate integrals in (27) and (33) now are given by

$$\Omega_0\big(y;f(\cdot)\big) = \int_{\mathbb{R}^m}\delta\left(z-\gamma\right)\phi(z)dz = \phi(\gamma), \tag{37}$$

and

$$\int_{\mathbb{R}^m}\delta\left(z-\gamma\right)H_{\mathbf{n}(\mathbf{\ddot{\imath}})-2\mathbf{a}+\mathbf{b_r}}\left(z\right)\phi(z)dz = H_{\mathbf{n}(\mathbf{\ddot{\imath}})-2\mathbf{a}+\mathbf{b_r}}(\gamma)\phi(\gamma). \tag{38}$$

Thus we obtain an explicit recursive formulas for the expansion coefficients $\Omega_k\big(\delta(\cdot-\gamma);y\big)$ presented in Theorem 4.1 below.

Theorem 4.1. *The expansion coefficient* $\Omega_k\big(\delta(\cdot-\gamma);y\big)$ *in* (33)*is explicitly given by*

$$\begin{aligned}\Omega_k\big(y;\delta(\cdot-\gamma)\big)=&\phi(\gamma)\sum_{(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k}\frac{1}{l!}\sum_{\boldsymbol{r}\in\{1,2,\ldots,m\}^l}\sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1}\\ \omega=1,\cdots,l}}\left(\prod_{\omega=1}^{l}C^{Y}_{\mathbf{i}_\omega,r_\omega}(y)\right)\\&\cdot\sum_{0\leq\boldsymbol{a}\leq\lfloor\mathbf{n}(\ddot{\boldsymbol{i}})/2\rfloor}\frac{\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{i}}}}{(\ell(\ddot{\boldsymbol{i}})-|\boldsymbol{a}|)!}H_{\mathbf{n}(\ddot{\boldsymbol{i}})-2\boldsymbol{a}+\boldsymbol{b_r}}(\gamma)\,,\end{aligned}\tag{39}$$

where $\boldsymbol{r}:=(r_1,\ldots,r_l)$, $\boldsymbol{b_r}:=\sum_{\omega=1}^{l}e_{r_\omega}$, $\gamma:=(y'-y)/\sqrt{t'-t}$, $\phi(\gamma)$ *is the m-dimensional standard normal density function and* $H_h(\gamma)$ *denotes its corresponding multivariate Hermite polynomial,* $\mathcal{S}_k$, $\mathcal{M}_j$, $C^{Y}_{\mathbf{i}_\omega,r_\omega}(y)$ *and* $\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{i}}}$ *are recursively defined by* (24), (15), (18) *and* (31), *respectively.*

By (25), (37) and (39), we obtain an explicit expression based on Hermite polynomials for the L-th order expansion of Li (2013) for the transition density of Y (cf. Equation (3.21) of Li (2013)):

$$p_Y^{(L,LI)}(t',y'|t,y)=\Delta^{-\frac{m}{2}}\phi(\gamma)+\Delta^{-\frac{m}{2}}\sum_{k=1}^{L}\Delta^{\frac{k}{2}}\Omega_k\big(y;\delta(\cdot-\gamma)\big),\tag{40}$$

and the true transition density $p_Y(t',y'|t,y)$ admits

$$p_Y(t',y'|t,y)=p_Y^{(L,LI)}(t',y'|t,y)+\mathcal{O}(\Delta^{\frac{L+1-m}{2}}).\tag{41}$$

Unlike the algorithms in Li (2013) and Li et al. (2016), the newly derived formula is explicitly expressed as a linear combination of Hermite polynomials, which allows us to connect it with the Hermite expansion and establish the equivalence result.

4.2 Recalculate formulas for the Hermite expansion of Yang et al. (2019) and Wan and Yang (2021)

In this subsection, we apply the pathwise expansion method to recompute the coefficients of the Hermite expansion, Equation (28) in Wan and Yang (2021), or equivalently Equation (22) in Yang et al. (2019) for the transformed diffusion Y.

For the process Y defined in (4), Wan and Yang (2021) expands the transition density $p_Y(t', y'|t, y)$ around $\phi(\gamma)$ to get the following expansion:

$$p_Y^{(J)}(t', y'|t, y) := \Delta^{-\frac{m}{2}}\phi(\gamma) + \Delta^{-\frac{m}{2}}\phi(\gamma)\sum_{j=1}^{J}\sum_{|h|=j}\eta^{(h)}(\Delta|t, y)\cdot H_h(\gamma), \tag{42}$$

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

$$\eta^{(h)}(\Delta|t, y) = \frac{1}{h!}\mathbb{E}\left[H_h\left(\frac{Y(t+\Delta) - y}{\sqrt{\Delta}}\right)\middle| Y(t) = y\right]. \tag{43}$$

In Theorem 2.1 of Wan and Yang (2021)), they show that the error of the expansion is of order $\mathcal{O}(\Delta^{(L+1-m)/2})$ when $J = 3L$, that is,

$$p_Y(t', y'|t, y) = p_Y^{(3L)}(t', y'|t, y) + \mathcal{O}(\Delta^{\frac{L+1-m}{2}}).$$

Furthermore, computing the coefficients $\eta^{(h)}$ of (43) in $p_Y^{(3L)}$ of (42) via the Itô-Taylor expansion method up to the order of $\mathcal{O}(\Delta^{L/2})$, that is

$$\eta^{(h)}(\Delta|t, y) = \eta_L^{(h)}(\Delta|t, y) + \mathcal{O}(\Delta^{\frac{L+1}{2}}), \tag{44}$$

and replacing $\eta^{(h)}$ with $\eta_L^{(h)}$ in (42) for $J = 3L$, they arrive at the L-th order *reduced Hermite expansion*; see Equation (28) of Wan and Yang (2021).

Next, we recalculate the Hermite expansion coefficient $\eta^{(h)}$ of (43) in $p_Y^{(3L)}$ of (42) using the pathwise expansion method up to the same order $\mathcal{O}(\Delta^{L/2})$. This allows us to derive an alternative expression for the reduced Hermite expansion of Wan and Yang (2021).

Recalling the conditional expectation defined in (9) and the Hermite expansion coefficient $\eta^{(h)}$ given by (43), and taking

$$f(\cdot) = H_h(\cdot), \tag{45}$$

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 (27) and (33) now are given by

$$\Omega_0\big(y; H_h(\cdot)\big) = \int_{\mathbb{R}^m} H_h(z)\,\phi(z)dz = \mathbf{1}_{\{h=0\}}, \tag{46}$$

and

$$\int_{\mathbb{R}^m} H_h\left(z\right) H_{\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}+\mathbf{b_r}}\left(z\right) \phi(z)dz = h! \cdot \mathbf{1}_{\{\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}+\mathbf{b_r}=h\}}. \tag{47}$$

Thus by (25), for $h = (h_1, h_2, \cdots, h_m) \in \mathbb{Z}_+^m$, the coefficients $\eta^{(h)}$ in (43) can be expanded as follows

$$\begin{aligned}\eta^{(h)}(\Delta|t,y) &= \frac{1}{h!}\Omega_0\big(y; H_h(\cdot)\big) + \frac{1}{h!}\sum_{k=1}^{L}\Omega_k\big(y; H_h(\cdot)\big)\epsilon^k + \mathcal{O}(\Delta^{\frac{L+1}{2}}) \\ &= \frac{1}{h!}\sum_{k=1}^{L}\Omega_k\big(y; H_h(\cdot)\big)\Delta^{\frac{k}{2}} + \mathcal{O}(\Delta^{\frac{L+1}{2}}),\end{aligned} \tag{48}$$

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

Theorem 4.2. *Given $h = (h_1, h_2, \cdots, h_m) \in \mathbb{Z}_+^m$, the expansion coefficient $\Omega_k\big(y; H_h(\cdot)\big)$ in (48) is explicitly given by*

$$\begin{aligned}\Omega_k(y; H_h(\cdot)) = \sum_{(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k} \frac{1}{l!} \sum_{\boldsymbol{r}\in\{1,2,\ldots,m\}^l} \sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1} \\ \omega=1,\cdots,l}} \left(\prod_{\omega=1}^{l} C^Y_{\mathbf{i}_\omega,r_\omega}(y)\right) \\ \cdot \frac{\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{\imath}}}}{(\ell(\ddot{\boldsymbol{\imath}}) - |\boldsymbol{a}|)!} \cdot h! \cdot \mathbf{1}_{\left\{\boldsymbol{a} = \frac{\mathbf{n}(\ddot{\boldsymbol{\imath}})+\boldsymbol{b_r}-h}{2},\ \boldsymbol{a}\in\mathbb{Z}^m\right\}},\end{aligned} \tag{49}$$

where $\boldsymbol{r} := (r_1, \ldots, r_l)$, $\boldsymbol{b_r} := \sum_{\omega=1}^{l} e_{r_\omega}$, $\mathcal{S}_k$, $\mathcal{M}_j$, $C^Y_{\mathbf{i}_\omega,r_\omega}(y)$ and $\tilde{w}_{\boldsymbol{a},\ddot{\boldsymbol{\imath}}}$ are recursively defined by (24), (15), (18) and (31), respectively.

Truncating the coefficient $\eta^{(h)}$ in (48) at the order $\Delta^{\frac{L}{2}}$, and plugging it into (42) for $J = 3L$, using the formula (49) for $\Omega_k\big(y; H_h(\cdot)\big)$, we get an alternative expression for the L-th order reduced Hermite expansion of Wan and Yang (2021) as follows,

$$p_Y^{(L,WY)}(t', y'|t, y) = \Delta^{-\frac{m}{2}}\phi(\gamma) + \Delta^{-\frac{m}{2}}\phi(\gamma)\sum_{j=1}^{3L}\sum_{|h|=j}\frac{1}{h!}\sum_{k=1}^{L}\Omega_k\big(y; H_h(\cdot)\big)\Delta^{\frac{k}{2}} \cdot H_h(\gamma). \tag{50}$$

4.3 Equivalence for the transformed diffusion Y

With the newly derived formulas in Theorems 4.1 and 4.2, the theorem below shows that the L-th order pathwise expansion of Li (2013) coincides with the L-th order reduced Hermite expansion of Wan and Yang (2021) or Yang et al. (2019) for the transformed diffusion Y.

Theorem 4.3. *For the transformed diffusion process Y defined in (4), we have*

$$p_Y^{(L,LI)}(t', y'|t, y) = p_Y^{(L,WY)}(t', y'|t, y), \tag{51}$$

where $p_Y^{(L,LI)}(t',y'|t,y)$ *is given by* (40) *and* (39)*, and* $p_Y^{(L,WY)}(t',y'|t,y)$ *is given by* (50) *and* (49)*.*

5 Equivalence of density expansions for the original diffusion X

In this section, we establish the equivalence result of the pathwise expansion of Li (2013) and the Hermite expansion of Wan and Yang (2021) or Yang et al. (2019) for the original diffusion X. We achieve this by utilizing the Jacobian formula for the change of density and the equivalence result for the transformed diffusion process Y.

5.1 Explicit alternative formulas of Li (2013)'s pathwise expansion for the original diffusion X

To return to the density expansion for the original diffusion, we can define $p_X^{(L,LI)}$ below via $p_Y^{(L,LI)}$ of (40) and (39) developed in Section 4.1:

$$p_X^{(L,LI)}(t',x'|t,x) := \det(\nu_0)^{-1/2}\, p_Y^{(L,LI)}(t',\nu_0^{-1/2}x'|t,\nu_0^{-1/2}x). \tag{52}$$

The proposition below demonstrates that $p_X^{(L,LI)}$ defined in (52) is exactly equivalent to Li (2013)'s density expansion for the original process X, denoted by $\tilde{p}_X^{(L,LI)}$. As a result, $p_X^{(L,LI)}$ defined in (52) is an explicit alternative formulas for Li (2013)'s pathwise expansion for the original diffusion X. The advantage of $p_X^{(L,LI)}$ in (52) is that it does not involve the conditional expectation of the multiplication of iterated Stratonovich integrals and their derivatives in Equation (3.26) of Li (2013).

Proposition 5.1. *The two expansions* $p_X^{(L,LI)}$ *defined in* (52) *and* $\tilde{p}_X^{(L,LI)}$ *provided by Equation (3.21) and (3.25) of Li (2013) are the same, that is,*

$$p_X^{(L,LI)}(t',x'|t,x) = \tilde{p}_X^{(L,LI)}(t',x'|t,x). \tag{53}$$

5.2 Equivalence for the original diffusion X

Similar to (52), we also define the Hermite expansion $p_X^{(L,WY)}$ for the original process X via the Hermite expansion $p_Y^{(L,WY)}$ of (50) and (49) developed in Section 4.2:

$$p_X^{(L,WY)}(t',x'|t,x) := \det(\nu_0)^{-1/2}\, p_Y^{(L,WY)}(t',\nu_0^{-1/2}x'|t,\nu_0^{-1/2}x). \tag{54}$$

Note that $p_Y^{(L,WY)}$ of (50) and (49) is an alternative formula for the (reduced) Hermite expansion (28) in Wan and Yang (2021) for the transformed process Y. Consequently $p_X^{(L,WY)}$ defined in (54) is an alternative formula for the Hermite expansion (32) in Wan and Yang (2021) for the original process X.

On one hand, we show in Section 4.3 that for the transformed diffusion Y, Li (2013)'s pathwise expansion $p_Y^{(L,LI)}(t', y'|t, y)$ given by (40) and (39) is identical to the Hermite expansion $p_Y^{(L,WY)}(t', y'|t, y)$ given by (50) and (49). Hence, when we backtrack to the original process X, we can see that $p_X^{(L,LI)}$ defined through (52) is the same as the Hermite expansion $p_X^{(L,WY)}$ defined through (54). On the other hand, we prove in Proposition 5.1 that $p_X^{(L,LI)}$ defined in (52) is identical to Li (2013)'s density expansion for the original process X. Consequently, we establish the equivalence between Li (2013)'s pathwise expansion and Wan and Yang (2021)'s Hermite expansion for the original process X.

Furthermore, Wan and Yang (2021) prove that the Hermite expansion $p_X^{(L,WY)}$ in (54) is the same as the delta expansion of Yang et al. (2019) for the transition density of the original process X under the choice of $\mu_0 = 0$. In conclusion, we summarize the equivalence result in the following theorem:

Theorem 5.1. *For a multivariate diffusion X defined in* (1)*, the pathwise expansion* (3.21) *in Li (2013), and the Hermite expansion* (32) *in Wan and Yang (2021) (or equivalently* (22) *in Yang et al. (2019) under the choice of $\mu_0 = 0$) have the same formulas.*

6 Concluding Remarks

In this paper, we derive explicit formulas for the conditional expectation of the pathwise Taylor expansion of a "general function" on a transformed diffusion. To achieve this, we employ a quasi-Lamperti transform to unify the process' diffusion matrix at the initial time, and we also utilize explicit expressions for the conditional expectation of the multiplication of iterated Itô integrals. The obtained result is new in the literature, providing a solution to the challenging problem of finding explicit formulas for the pathwise Taylor expansion.

Using the above result, we show the equivalence of different transition densities expansions existing in the literature. Initially, we apply the method to recalculate density expansions based on the pathwise expansion method of Li (2013) and the Hermite expansion of Yang et al.

(2019) and Wan and Yang (2021) for the transformed diffusion. The newly derived formulas in both cases are expressed in terms of Hermite polynomials. By rearranging the terms in the density expansions according to the increasing order of the Hermite polynomials, we establish the equivalence between the two methods for the transformed process. Subsequently, we utilize the Jacobian formula to perform a change of variable from the transformed process to the original process, thereby establishing the connections between the two expansion methods for the original process. This enables us to refer to both of them as *the Hermite expansion method*. Furthermore, we can conveniently implement the relatively simple expression for *the Hermite expansion method*, as presented in Equation (22) by Yang et al. (2019).

In addition, the explicit formulas for the conditional expectation of the pathwise Taylor expansion has wide-ranging applications in various areas. They are particular useful for finding small-time approximations of functionals of multivariate diffusion process, including option prices, moment generating functions, and various statistics, among others. These topics offer exciting prospects for future research.

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A The Proofs

Proof of Theorem 3.1. Recall the coefficient $\Phi_k\big(y; f(\cdot)\big)$ in (22):

$$\Phi_k\big(y; f(\cdot)\big) = \sum_{(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k} \sum_{\mathbf{r}\in\{1,2,\ldots,m\}^l} \frac{1}{l!}\partial_z^{\mathbf{b}_\mathbf{r}} f(z)\Big|_{z=W(1)} \prod_{\omega=1}^{l} F^Y_{j_\omega+1,r_\omega}, \tag{55}$$

with $\mathbf{r} := (r_1, \ldots, r_l)$, $\mathbf{b}_\mathbf{r} := \sum_{\omega=1}^{l} e_{r_\omega}$, $\mathcal{S}_k$ is given by (24), and $F^Y_{j_\omega+1}$ is given by (17).

To compute the expectation $\Omega_k\big(y; f(\cdot)\big) = \mathbb{E}[\Phi_k\big(y; f(\cdot)\big)]$ defined in (26), using integration by parts formula, we have

$$\mathbb{E}\Big[\partial_z^{\mathbf{b_r}} f(z)\Big|_{z=W(1)} \prod_{\omega=1}^{l} F^Y_{j_\omega+1,r_\omega}\Big] = \int_{\mathbb{R}^m} \partial_z^{\mathbf{b_r}} f(z) \left(\mathbb{E}\Big[\prod_{\omega=1}^{l} F^Y_{j_\omega+1,r_\omega} | W(1)=z\Big]\phi(z)\right) dz$$
$$=(-1)^l \int_{\mathbb{R}^m} f(z)\, \partial_z^{\mathbf{b_r}} \left(\mathbb{E}\Big[\prod_{\omega=1}^{l} F^Y_{j_\omega+1,r_\omega} | W(1)=z\Big]\phi(z)\right) dz, \tag{56}$$

where we have used the fact that $|\mathbf{b_r}| = l$. The conditional expectation is given by (cf. (17))

$$\mathbb{E}\left[\prod_{\omega=1}^{l} F^Y_{j_\omega+1,r_\omega} \middle| W(1)=z\right] = \sum_{\substack{\mathbf{i}_\omega \in \mathcal{M}_{j_\omega+1} \\ \omega=1,\cdots,l}} \left(\prod_{\omega=1}^{l} C^Y_{\mathbf{i}_\omega, r_\omega}(y) \cdot \mathbb{E}\left[\prod_{\omega=1}^{l} \mathbb{I}_{\mathbf{i}_\omega}(1) \middle| W(1)=z\right]\right), \tag{57}$$

where $C^Y_{\mathbf{i}_\omega, r_\omega}(y)$ is given by (18), and $\mathcal{M}_j$ is recursively defined by (15). By Lemma 3.2,

$$\mathbb{E}\left[\prod_{\omega=1}^{l} \mathbb{I}_{\mathbf{i}_\omega}(1) \middle| W(1)=z\right] = \sum_{0 \le \mathbf{a} \le \lfloor \mathbf{n}(\ddot{\mathbf{i}})/2 \rfloor} \frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}}) - |\mathbf{a}|)!} H_{\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}}(z). \tag{58}$$

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

$$(-1)^l \partial_z^{\mathbf{b_r}} \left(H_{\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}}(z)\, \phi(z)\right) = (-1)^{l+|\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}|} \partial_z^{\mathbf{b_r}+\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}} \phi(z) = H_{\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}+\mathbf{b_r}}(z)\, \phi(z). \tag{59}$$

Plugging (57), (58) and (59) into (56), we have

$$\mathbb{E}\Big[\partial_z^{\mathbf{b_r}} H_h(z)\Big|_{z=W(1)} \prod_{\omega=1}^{l} F^Y_{j_\omega+1,r_\omega}\Big]$$
$$= \sum_{\substack{\mathbf{i}_\omega \in \mathcal{M}_{j_\omega+1} \\ \omega=1,\cdots,l}} \left(\prod_{\omega=1}^{l} C^Y_{\mathbf{i}_\omega, r_\omega}(y)\right) \sum_{0 \le \mathbf{a} \le \lfloor \mathbf{n}(\ddot{\mathbf{i}})/2 \rfloor} \frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}}) - |\mathbf{a}|)!} \cdot \int_{\mathbb{R}^m} H_h(z)\, H_{\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}+\mathbf{b_r}}(z)\, \phi(z) dz.$$

Then, the proposition is proved by substituting the above equation into the expectation of (55). □

Proof of Theorem 4.3. As the reduced Hermite expansion $p_Y^{(L,WY)}(t', y'|t, y)$ given by (50) and (49) is arranged according to the increasing order of the Hermite polynomials. To compare with it, we first show that the pathwise expansion $p_Y^{(L,LI)}(t', y'|t, y)$ given by (40) and (39) can also be rearranged according to the increasing order of the Hermite polynomials as follows:

$$p_Y^{(L,LI)}(t', y'|t, y) = \Delta^{-\frac{m}{2}} \phi(\gamma) + \Delta^{-\frac{m}{2}} \phi(\gamma) \sum_{j=1}^{3L} \sum_{|h|=j} \eta^{(h,LI)}(\Delta|t, y) \cdot H_h(\gamma), \tag{60}$$

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

$$\eta^{(h,LI)}(\Delta|t,y)=\sum_{k=1}^{L}\Delta^{\frac{k}{2}}\sum_{(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k}\frac{1}{l!}\sum_{\mathbf{r}\in\{1,2,\ldots,m\}^l}\sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1}\\ \omega=1,\cdots,l}}\left(\prod_{\omega=1}^{l}C^{Y}_{\mathbf{i}_\omega,r_\omega}(y)\right)$$
$$\cdot\frac{\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}}{(\ell(\ddot{\mathbf{i}})-|\mathbf{a}|)!}\cdot\mathbf{1}_{\{\mathbf{a}=\frac{\mathbf{n}(\ddot{\mathbf{i}})+\mathbf{b_r}-h}{2},\mathbf{a}\in\mathbb{Z}^m\}}. \tag{61}$$

Here, $\mathbf{r}:=(r_1,\ldots,r_l)$, $\mathbf{b_r}:=\sum_{\omega=1}^{l}e_{r_\omega}$, $\phi(\gamma)$ and $H_h(\gamma)$ are the m-dimensional standard normal density function and the corresponding multivariate Hermite polynomial, respectively; $\mathcal{S}_k$, $\mathcal{M}_j$, $C^{Y}_{\mathbf{i}_\omega,r_\omega}(y)$ and $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$ are recursively defined by (24), (15), (18) and (31), respectively.

If (60) with (61) holds, comparing the formula $\Omega_k(y;H_h(\cdot))$ in (49) and $\eta^{(h,LI)}(\Delta|t,y)$ in (61), we have

$$\eta^{(h,LI)}(\Delta|t,y)=\frac{1}{h!}\sum_{k=1}^{L}\Omega_k(y;H_h(\cdot))\Delta^{\frac{k}{2}}. \tag{62}$$

Plugging (62) into (60), and comparing the result with (50), the theorem is proved.

Now, we begin to prove (60) with (61). According to the definition of the coefficient $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$ in Lemma 3.2, $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}=0$ if $\min(\mathbf{a})<0$ or $\max(2\mathbf{a}-\mathbf{n}(\ddot{\mathbf{i}}))>0$. Thus, we can take summation for $\mathbf{a}$ over all m-dimensional integers in (39). Plugging it into (40), we have

$$p_Y^{(L,LI)}(t',y'|t,y)=\Delta^{-\frac{m}{2}}\phi(\gamma)+\Delta^{-\frac{m}{2}}\phi(\gamma)\sum_{k=1}^{L}\Delta^{\frac{k}{2}}\sum_{(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k}\frac{1}{l!}\sum_{\mathbf{r}\in\{1,2,\ldots,m\}^l}\sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1}\\ \omega=1,\cdots,l}}$$
$$\cdot\left(\prod_{\omega=1}^{l}C^{Y}_{\mathbf{i}_\omega,r_\omega}(y)\right)\sum_{\mathbf{a}\in\mathbb{Z}^m}\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}\cdot\frac{1}{(\ell(\ddot{\mathbf{i}})-|\mathbf{a}|)!}H_{\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}+\mathbf{b_r}}(\gamma). \tag{63}$$

Consider the following change of variable:

$$h=\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}+\mathbf{b_r}. \tag{64}$$

Note that in (64) each component of $\mathbf{n}(\ddot{\mathbf{i}})+\mathbf{b_r}-h$ is even, or $\mathbf{a}:=(\mathbf{n}(\ddot{\mathbf{i}})+\mathbf{b_r}-h)/2$ is an integer-valued vector, i.e., $\mathbf{a}\in\mathbb{Z}^m$. Thus, (63) becomes (for simplification, below we still use both h and $\mathbf{a}$ satisfying the relationship (64))

$$p_Y^{(L,LI)}(t',y'|t,y)=\Delta^{-\frac{m}{2}}\phi(\gamma)+\Delta^{-\frac{m}{2}}\phi(\gamma)\sum_{k=1}^{L}\Delta^{\frac{k}{2}}\sum_{(j_1,j_2,\ldots,j_l)\in\mathcal{S}_k}\frac{1}{l!}\sum_{\mathbf{r}\in\{1,2,\ldots,m\}^l}\sum_{\substack{\mathbf{i}_\omega\in\mathcal{M}_{j_\omega+1}\\ \omega=1,\cdots,l}}$$
$$\cdot\left(\prod_{\omega=1}^{l}C^{Y}_{\mathbf{i}_\omega,r_\omega}(y)\right)\sum_{h\in\mathbb{Z}^m}\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}\cdot\frac{1}{(\ell(\ddot{\mathbf{i}})-|\mathbf{a}|)!}H_h(\gamma)\cdot\mathbf{1}_{\{h=\mathbf{n}(\ddot{\mathbf{i}})-2\mathbf{a}+\mathbf{b_r},\mathbf{a}\in\mathbb{Z}^m\}}. \tag{65}$$

Interchanging the order of summation with respect to k and h leads to (please refer to (61) for the definition of $\eta^{(h,LI)}$)

$$p_Y^{(L,LI)}(t',y'|t,y) = \Delta^{-\frac{m}{2}}\phi(\gamma) + \Delta^{-\frac{m}{2}}\phi(\gamma)\sum_{h\in\mathbb{Z}^m} H_h(\gamma)\,\eta^{(h,LI)}(\Delta|t,y). \tag{66}$$

Then, we get (60) by recalling the definition of $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$. Indeed, to get a non-zero $\tilde{w}_{\mathbf{a},\ddot{\mathbf{i}}}$, it requires that

$$0 \leq 2\mathbf{a} \equiv \mathbf{n}(\ddot{\mathbf{i}}) + \mathbf{b_r} - h \leq \mathbf{n}(\ddot{\mathbf{i}}) \Leftrightarrow \mathbf{b_r} \leq h \leq \mathbf{n}(\ddot{\mathbf{i}}) + \mathbf{b_r}. \tag{67}$$

Noting that $|\mathbf{b_r}| = l$, and for $\ddot{\mathbf{i}} := \{\mathbf{i}_1, \cdots, \mathbf{i}_l\}$ and $\mathbf{i}_\omega \in \mathcal{M}_{j_\omega+1}, \omega = 1, \cdots, l$, and recalling the definition of $\mathcal{M}_{j_\omega+1}$ and $\mathcal{S}_k$ in (14) and (23) respectively, then we have

$$\begin{aligned}|\mathbf{n}(\ddot{\mathbf{i}})| &:= \sum_{\alpha=1}^{m} n_{\ddot{\mathbf{i}}}(\alpha) = \sum_{\omega=1}^{l}\sum_{\alpha=1}^{m} n_{\mathbf{i}_\omega}(\alpha) = \sum_{\omega=1}^{l}(||\mathbf{i}_\omega|| - 2n_{\mathbf{i}_\omega}(0)) \\ &= \sum_{\omega=1}^{l}(j_\omega + 1) - 2n_{\ddot{\mathbf{i}}}(0) = k + l - 2n_{\ddot{\mathbf{i}}}(0).\end{aligned} \tag{68}$$

Furthermore, for $1 \leq k \leq L$ and $(j_1, j_2, \ldots, j_l) \in \mathcal{S}_k$, we have that $1 \leq l \leq k \leq L$. Then, combining (67) and (68), we have

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

This proves that (60) with (61) holds. The proof is finished. □

Proof of Proposition 5.1. Noting (11) and (35), the quasi-Lamperti transform (3), and the Jacobian formula for the change of variable lead to the transition density of X below:

$$p_X(t',x'|t,x) = \Delta^{-\frac{m}{2}}\det(\nu_0)^{-1/2}\,\mathbb{E}\left[\delta\left(\Gamma^\epsilon - \gamma\right)\Big|Y(t) = y\right], \tag{69}$$

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 $p_X^{(L,LI)}(t',x'|t,x)$ given in (52) is the L-th order Taylor expansion of the right hand side of (69) with respect to ϵ.

On the other hand, Li (2013) characterizes the transition density of X as following

$$p_X(t',y'|t,y) = \Delta^{-\frac{m}{2}}\det(D(x))\mathbb{E}[\delta(\widetilde{Y}^\epsilon - \widetilde{y})|X(t) = x] \tag{70}$$

where $D(x)$ is a diagonal matrix given by Equation (3.12) in Li (2013):

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

$\widetilde{Y}^\epsilon := D(x)(X^\epsilon(1) - x)/\epsilon$, and $\widetilde{y} = D(x)(x' - x)/\epsilon$. The expansion $\tilde{p}_X^{(L,LI)}$ provided by Equation (3.21) and (3.25) of Li (2013) is the L-th order Taylor expansion of the right hand side of (70) 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 side of (69) and (70) are identical. Thus, the proposition is proved. □

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