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### Closed-Form Expansion, Conditional Expectation, and Option Valuation

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Enlightened by the theory of Watanabe [Watanabe S (1987) Analysis of Wiener functionals (Malliavin calculus) and its applications to heat kernels. Ann. Probab. 15:1-39] for analyzing generalized random variables and its further development in Yoshida [Yoshida N (1992a) Asymptotic expansions for statistics related to small diffusions. J. Japan Statist. Soc. 22: 139–159], Takahashi [Takahashi A (1995) Essays on the valuation problems of contingent claims. Ph.D. thesis, Haas School of Business, University of California, Berkeley, Takahashi A (1999) An asymptotic expansion approach to pricing contingent claims. Asia-Pacific Financial Markets 6:115–151] as well as Kunitomo and Takahashi [Kunitomo N, Takahashi A (2001) The asymptotic expansion approach to the valuation of interest rate contingent claims. Math. Finance 11(1):117-151, Kunitomo N, Takahashi A (2003) On validity of the asymptotic expansion approach in contingent claim analysis. Ann. Appl. Probab. 13(3):914–952] etc., we focus on a wide range of multivariate diffusion models and propose a general probabilistic method of small-time asymptotic expansions for approximating option price in simple closed-form up to an arbitrary order. To explicitly construct correction terms, we introduce an efficient algorithm and novel closed-form formulas for calculating conditional expectation of multiplication of iterated stochastic integrals, which are potentially useful in a wider range of topics in applied probability and stochastic modeling for operations research. The performance of our method is illustrated through various models nested in constant elasticity of variance type processes. With an application in pricing options on VIX under GARCH diffusion and its multifactor generalization to the Gatheral double lognormal stochastic volatility models, we demonstrate the versatility of our method in dealing with analytically intractable non-Lévy and non-affine models. The robustness of the method is theoretically supported by justifying uniform convergence of the expansion over the whole set of parameters.

*Key words*: asymptotic expansion; diffusion; option pricing; conditional expectation; iterated stochastic integral *MSC2000 subject classification*: Primary: 91G60, 91B70; secondary: 60H30, 91G80 *OR/MS subject classification*: Primary: asset pricing, diffusion, stochastic model applications *History*: Received July 2, 2010; revised March 18, 2012, November 22, 2012, and May 18, 2013. Published online in *Articles in Advance.* 

**1. Introduction.** Modeling and pricing of increasingly sophisticated derivative securities are central to financial engineering. Modeling is usually a trade-off between mathematical tractability and empirical performance. To explain and fit market trading data, however, increasingly more recent research indicates that some analytically tractable models may not be able to render satisfactory empirical performance compared with those having less mathematical tractability. For instance, Christoffersen et al. [14] have demonstrated the superior empirical features of the GARCH diffusion specification of stochastic volatility over the well-known square- root specification proposed in Heston [36] for modeling the volatility of S&P500 index returns. Also, Gatheral [27] has shown that the double lognormal specification of stochastic volatility outperforms the double Heston type specification for modeling options on VIX (the CBOE implied volatility index, see CBOE [12]). However, both the GARCH diffusion and the double lognormal stochastic volatility models belong to the large family of non-Lévy and non-affine diffusions (see Dai and Singleton [18]), for which characteristic functions do not exist in closed form. Thus, most analytical methods (e.g., the Fourier or Laplace transform inversions) heavily relying on analytical tractability of the models are not applicable. Therefore, the closed-form asymptotic expansion method becomes a viable option for providing flexible, efficient, and easy-to-implement solutions.

From a technical perspective, asymptotic expansions have become prevalent in option valuation owing to their efficiency and flexibility. Among others, a well-known method is based on perturbations of partial differential equations (hereafter PDE); see, e.g., Hagan et al. [33], Andersen and Brotherton-Ratcliffe [3], Fouque et al. [25, 26], Takahashi and Yamada [69], and Kato et al. [44]. Another attractive approach is a probabilistic method based on the theory for analyzing generalized Wiener functionals (random variables) initiated by Watanabe [74] and its substantial development in favor of a small-diffusion setting (by parameterizing an auxiliary parameter only in diffusion components of underlying models) for statistical inference and option valuation in, e.g., Yoshida [76], Takahashi [61, 62], Kunitomo and Takahashi [48, 49], and Osajima [57]. Resorting to calculation of the first several orders of the expansions, various applications can also be found in, e.g., Kunitomo and Takahashi [47], Uchida and Yoshida [72], Takahashi and Takehara [64, 65], Takahashi [63], Takahashi and Yamada [70], Takahashi and Toda [68], Kawai [45], Jaeckel and Kawai [40], Gobet et al. [30, 31], and Márquez-Carreras and Sanz-Solé [52].

However, to achieve better accuracy, robustness, and reliability and to make the implementation as comparably convenient as that of Monte Carlo simulation, seeking for relatively simple closed-form formulas or computationally efficient algorithms in order to symbolically implement high-order correction terms has become one of the major tasks for various asymptotic expansion methods. Among many others, at a level of generality and an expense of complexity, a recursion-based framework regardless of particular types of parameterization is outlined in Takahashi et al. [66, 67] with emphasis on small-diffusion type expansion aiming at the valuation of options with relatively long maturities. As an indispensable development of the asymptotic expansion methods, we will alternatively focus on small-time type expansion, which has become an important analytical method in financial engineering because of its simplicity and the concrete economic interpretations; see, e.g., Hagan and Woodward [34], Hagan et al. [33], Andersen and Brotherton-Ratcliffe [3] and Section 10 in Lipton [50] for approximating option prices via PDE-based perturbation methods as well as Takahashi and Yamada [69] for approximating heat kernels via the integration-by-parts techniques of Malliavin calculus; see, e.g., chapter 1 in Nualart [55].

Focusing on a wide range of diffusion models, we will propose a general closed-form formula (with only basic mathematical operations without recursions or integrations) up to an arbitrary order for small-time expansion of option price via a probabilistic approach. The application of Itô-Stratonovich stochastic calculus and the theory of Watanabe [74] leads to the analytical tractability, Simplicity, and versatility of our closed-form expansion, particularly for some sophisticated models, in which small-diffusion expansions involve numerically solving ordinary differential equations and calculating integrals owing to the complexity of drift and diffusion functions; see, e.g., the nonlinear stochastic variance and nonlinear drift model for spot interest rates and variance proposed and investigated in Aït-Sahalia [1] and Bakshi et al. [4]. To pragmatically build any arbitrary closed-form expansion of iterated Stratonovich integrals driven by multidimensional Brownian motions. At the heart of this algorithm, we employ combinatorial analysis to establish a novel closed-form formula for computing conditional expectation of multiplication of iterated Itô integrals. These developments substantially generalize the existing results( see, e.g., Nualart et al. [56], Yoshida [76], Takahashi [61, 62], Kunitomo and Takahashi [48, 49], and Takahashi et al. [66, 67]) and are potentially useful in a wide range of studies in applied probability and stochastic modeling for operations research.

Without loss of generality, we demonstrate the performance of our method using the celebrated constant elasticity of variance (CEV) type process (see, e.g., Cox [16] and Davydov and Linetsky [19]), in which several commonly used models are nested. In addition, we apply our method in the valuation of options on VIX, which is a challenging issue in derivatives valuation. As a fundamental instrument for hedging, call options on VIX have become effective tools for managing downside risk. For instance, through rolling options on VIX with one-month maturity, the VXTH (VIX tail hedge) proposed in CBOE [13] has uniformly outperformed the S&P500 index during the financial depressions; see CBOE [13]. We apply our method to the valuation of options on VIX under the GARCH diffusion stochastic volatility model (see Christoffersen et al. [14]) and its multifactor extension to the Gatheral double lognormal model (see, e.g., Gatheral [27]). Such applications demonstrate the versatility of our method in dealing with analytically intractable non-Lévy and non-affine models as well as nonlinear payoff functions.

It is noteworthy that the convergence of our expansion can be guaranteed theoretically under some sufficient conditions on the specification of the underlying model. As shown in the computational results, however, the applicability of the expansions is not confined to the models, of which the sufficient conditions for convergence are strictly satisfied, but instead is extendable to a wide range of commonly used derivatives pricing models. Similar to other existing applications of small-time expansions (e.g., Andersen and Brotherton-Ratcliffe [3], Hagan and Woodward [34], Hagan et al. [33], and Takahashi and Yamada [69]) numerical illustrations suggest that our method does not necessarily require the option maturity to be small in order to deliver satisfactory performance. At least in principle, arbitrary accuracy could be obtained by employing high-order expansions based on our general formulas and algorithms. However, we note that, as demonstrated in the computational results given in §5, the performance of the expansions is reasonably model dependent.

The rest of this paper is organized as follows. In §2, we propose the model and a basic setup. In §3, we build up a general framework for obtaining closed-form asymptotic expansion up to an arbitrary order for option valuation. Section 4 is devoted to establishing algorithms and closed-form formulas for the computation of conditional expectation of multiplication of iterated stochastic integrals, which plays a central role in constructing the expansions. In §5, we demonstrate the performance of our method through several examples including the valuation of European options under various CEV type models, as well as the valuation of options on VIX under the GARCH diffusion and the Gatheral double lognormal stochastic volatility models. We conclude this paper in §6. The proofs are provided in Appendices A and B.

**2.** The model and basic setup. We consider a risk-neutral specification of a general multivariate diffusion model governed by the following stochastic differential equation (hereafter SDE):

$$dX(t) = \mu(X(t), \theta)dt + \sigma(X(t), \theta)dW(t), \quad X(0) = x_0 = (x_{01}, x_{02}, \dots, x_{0m}),$$
(1)

where X(t) is an *m*-dimensional vector of state variables;  $x_0 = (x_{01}, x_{02}, \ldots, x_{0m})$  is the initial state;  $\{W(t)\}$  is a *d*-dimensional standard Brownian motion;  $\theta$  represents a vector of model parameters belonging to a bounded open set  $\Theta$ ;  $\mu(x, \theta) = (\mu_1(x, \theta), \ldots, \mu_m(x, \theta))$  is an *m*-dimensional vector function; and  $\sigma(x, \theta) = (\sigma_{ij}(x, \theta))_{m \times d}$  is an  $m \times d$  matrix-valued function. For ease of exposition and without loss of generality, we assume that m = d and drop the parameter vector  $\theta$  throughout the rest of this paper. Let  $E(\subset R^m)$  denote the state space (all possible values) of X. Suppose the price of an underlying asset satisfies

$$S(t) = f(X(t)), \tag{2}$$

for some function f(x) sufficiently smooth in E with  $(\partial f/\partial x_1, \partial f/\partial x_2, \dots, \partial f/\partial x_m) \neq 0$ . Without loss of generality, we assume that  $\partial f/\partial x_1 \neq 0$ .

A simplest one-dimensional example is the celebrated Black-Scholes-Merton model (see Black and Scholes [6] and Merton [53]), for which the functions are specified as

$$f(x) = x,$$
  $\mu(x) = rx,$  and  $\sigma(x) = \sigma x$ 

for some positive constants r and  $\sigma$  representing the risk-free interest rate and constant volatility, respectively. Slightly more general in order to reflect the leverage effect between the asset return and its random volatility, the constant elasticity of variance model (see, e.g., Cox [16] and Davydov and Linetsky [19]) can be specified via

$$f(x) = x, \quad \mu(x) = rx, \quad \text{and} \quad \sigma(x) = \delta x^{\beta},$$
 (3)

for some constants  $\delta$  and  $\beta$ . Also, by setting

$$f((x_1, x_2)) = x_1, \qquad \mu((x_1, x_2)) = \begin{pmatrix} rx_1 \\ \mu_2(x_2) \end{pmatrix}, \qquad \text{and} \qquad \sigma((x_1, x_2)) = \begin{pmatrix} \sqrt{x_2}x_1 & 0 \\ \sigma_{21}(x_2) & \sigma_{22}(x_2) \end{pmatrix}$$

for some functions  $\mu_2(\cdot)$ ,  $\sigma_{21}(\cdot)$ , and  $\sigma_{22}(\cdot)$ , we create a model for incorporating stochastic volatility; see, e.g., Fouque et al. [25] and the references therein. In particular, by letting  $\mu_2(x_2) = \kappa(\theta - x_2)$  for some positive  $\kappa$ and  $\theta$ , we model the mean-reversion effect in the stochastic variance; by letting  $\sigma_{21}(x_2) = \rho\sqrt{x_2}$  and  $\sigma_{22}(x_2) = \sqrt{1 - \rho^2}\sqrt{x_2}$ , for some constant  $-1 \le \rho \le 1$ , we obtain the well-known Heston stochastic volatility model (see Heston [36]). Alternatively, by letting  $\sigma_{21}(x_2) = \rho x_2$  and  $\sigma_{22}(x_2) = \sqrt{1 - \rho^2} x_2$ , we build the GARCH diffusion stochastic volatility model, which is recently shown to be a popular candidate for empirically fitting the volatility of S&P500 returns; see, e.g., Christoffersen et al. [14] and Barone-Adesi et al. [5].

On a level of generality, we suppose that a derivative security pays out p(S(T)) for some payoff function p(x) at a maturity time T. Assuming the risk-free interest rate r to be a constant, the initial arbitrage-free price of this derivative is given by

$$V(0) := E[e^{-rT}p(S(T))] = E[e^{-rT}p(f(X(T)))].$$
(4)

Except for a limited number of mathematically tractable models, V(0) is usually calculated by various numerical methods such as Monte Carlo simulation, numerical methods of partial differential equations, and approximations by binomial (or multinomial) lattice. However, for efficient calibration of the model to market trading data, simple closed-form formulas or analytical approximations are preferred to avoid repeated calculations for optimization. In this paper, we propose an easy-to-implement method for calculating closed-form asymptotic expansion approximation for option valuation. Without loss of generality and for ease of exposition, we demonstrate our method via the valuation of a call option with a payoff function

$$p(x) := (x - K)^{+} \equiv \max(x - K, 0) \quad \text{for some strike } K.$$
(5)

Before closing this section, we introduce the following technical assumptions in order to guarantee the theoretical validity of our expansion. Let  $A(x) = \sigma(x)\sigma(x)^T = (a_{ij}(x))_{m \times m}$  denote the diffusion matrix.

ASSUMPTION 1. The diffusion matrix A(x) is positive definite, i.e., det A(x) > 0, for any x in E (the state space of the underlying diffusion X).

Assumption 2. For each integer  $k \ge 1$ , the kth order derivatives in x of the functions  $\mu(x; \theta)$  and  $\sigma(x; \theta)$  are uniformly bounded for any  $(x, \theta) \in E \times \Theta$ .

Assumption 3. For each integer  $k \ge 1$ , the kth order derivatives in x of the function f(x) are bounded in E.

Assumptions 1 and 2 are standard and conventionally proposed in the study of SDEs (see, e.g., Ikeda and Watanabe [38]). They are sufficient (but do not need to be necessary) to guarantee the existence and uniqueness of the solution and many other desirable technical properties. As shown in what follows, under these conditions, the theory of Watanabe [74] guarantees validity of the expansion discussed in this paper. Theoretical relaxation on these conditions may involve case-by-case treatments and standard approximation arguments, which is beyond the scope of this paper and can be regarded as a future research topic.

#### 3. Closed-form expansion for option valuation.

**3.1. Explicit path-wise expansion.** Inheriting the tradition of small-time expansions( see, e.g., the PDE based methods proposed in Andersen and Brotherton-Ratcliffe [3] and Takahashi and Yamada [69]) we choose  $\epsilon = \sqrt{T}$  as a parameter based on which the expansion is carried out. We begin with rescaling (1) as  $X^{\epsilon}(t) := X(\epsilon^2 t)$  in order to bring forth finer local behavior of the diffusion process. By integral substitutions and the Brownian scaling property, it follows that

$$dX^{\epsilon}(t) = \epsilon^{2} \mu(X^{\epsilon}(t))dt + \epsilon \sigma(X^{\epsilon}(t))dW^{\epsilon}(t), \qquad X^{\epsilon}(0) = x_{0}, \tag{6}$$

where  $\{W^{\epsilon}(t)\}\$  is a *m*-dimensional standard Brownian motion. To simplify notations, we will let W(t) denote the scaled Brownian motion  $W^{\epsilon}(t)$  in the rest of the paper.

We note that the general framework outlined in Takahashi et al. [66, 67] includes various methods of parametrization, e.g., the well-studied small-diffusion parametrization (see, e.g., Takahashi [61, 62, 63] and Uchida and Yoshida [72]) and (6). However, as further demonstrated in what follows, the small-time parameterization (6) leads to significant simplicity, explicity, and computational convenience. First, without need of the general recursion proposed in Takahashi et al. [66, 67], a path-wise expansion of  $X^{\epsilon}(t)$  can be obtained in a simple closed-form using appropriate differential operators and iterated Stratonovich integrals via the Itô-Stratonovich stochastic calculus. Thus, based on the theory of Watanabe [74], an expansion for option valuation can be explicitly given via proper indices combinations, which leads to convenient symbolic implementation. In this regard, our explicit expansion formula can be seen as an important closed-form solution to the recursion-based asymptotic expansion scheme proposed in Takahashi et al. [66, 67]. Second, as discussed in §§3.2 and 4, the conditional expectations involving iterated stochastic integrals, which centralize the explicit calculation of the expansions, are irrelevant of the specification of drift or diffusion. Compared with the small-diffusion expansions, this advantage facilitates the implementation of high-order expansions.

Instead of directly considering the parameterized SDE (6) like most of the existing expansion methods do, e.g., Takahashi et al. [66, 67], we focus on its equivalent Stratonovich form:

$$dX^{\epsilon}(t) = \epsilon^2 b(X^{\epsilon}(t))dt + \epsilon \sigma(X^{\epsilon}(t)) \circ dW(t), \tag{7}$$

where  $\circ$  denotes stochastic integrals in the Stratonovich sense and the vector-valued function  $b(x) = (b_1(x), b_2(x), \dots, b_m(x))^T$  is defined by

$$b_i(x) = \mu_i(x) - \frac{1}{2} \sum_{k=1}^m \sum_{j=1}^d \sigma_{kj}(x) \frac{\partial}{\partial x_k} \sigma_{ij}(x).$$
(8)

In our setting, Stratonovich integrals offer significant computational convenience compared with Itô integrals in that the Itô-Stratonovich formula resembles the chain rule in classical calculus (see, e.g., Section 3.3 in Karatzas and Shreve [43]), which will play an important role in constructing a simple closed-form expansion up to any arbitrary order.

A natural start is to expand  $f(X^{\epsilon}(1))$  as a series of  $\epsilon$  with random coefficients. Following the assumption of  $\partial f/\partial x_1 \neq 0$ , we further assume that there exists a function  $g: \mathbb{R}^m \to \mathbb{R}$  such that, for  $y_1 = f(x_1, x_2, \dots, x_m)$ , one has  $x_1 = g(y_1, x_2, \dots, x_m)$ . Thus, for computational convenience, we introduce a diffusion process  $Y^{\epsilon}(t) = (Y_1^{\epsilon}(t), Y_2^{\epsilon}(t), \dots, Y_m^{\epsilon}(t))$  defined by

$$Y_1^{\epsilon}(t) = f(X^{\epsilon}(t)) = f(X_1^{\epsilon}(t), X_2^{\epsilon}(t), \dots, X_m^{\epsilon}(t)), \qquad Y_2^{\epsilon}(t) = X_2^{\epsilon}(t), \dots, \qquad \text{and} \qquad Y_m^{\epsilon}(t) = X_m^{\epsilon}(t).$$
(9)

A straightforward application of the Itô-Stratonovich formula yields the following SDE for  $Y^{\epsilon}(t)$ :

$$dY^{\epsilon}(t) = \epsilon^{2} \alpha(Y^{\epsilon}(t)) dt + \epsilon \beta(Y^{\epsilon}(t)) \circ dW(t), \qquad Y^{\epsilon}(0) = y_{0} = (f(x_{01}, x_{02}, \dots, x_{0m}), x_{02}, \dots, x_{0m}),$$
(10)

where the drift vector function and the dispersion matrix are specified as follows: for  $y = (y_1, y_2, \dots, y_m)$ ,

$$\alpha(y) = \left(\sum_{i=1}^{m} \frac{\partial f}{\partial x_i}(g(y), y_2, \dots, y_m)b_i(g(y), y_2, \dots, y_m), b_2(g(y), y_2, \dots, y_m), \dots, b_m(g(y), y_2, \dots, y_m)\right)^T$$
(11)

and

$$\beta(y) = \left(\sum_{i=1}^{m} \frac{\partial f}{\partial x_i}(g(y), y_2, \dots, y_m) \sigma_i(g(y), y_2, \dots, y_m), \sigma_2(g(y), y_2, \dots, y_m), \dots, \sigma_m(g(y), y_2, \dots, y_m)\right)^T,$$
(12)

where  $\sigma_i$  denotes the *j*th row vector of the diffusion matrix  $\sigma$ . Here,  $\cdot^T$  denotes the transpose of a matrix.

Inheriting the idea from Watanabe [74] for constructing heat-kernel expansions, we introduce the following differential operators for expressing the expansion terms in simple closed form:

$$\mathcal{A}_{0} := \sum_{i=1}^{m} \alpha_{i}(y) \frac{\partial}{\partial y_{i}} \quad \text{and} \quad \mathcal{A}_{j} := \sum_{i=1}^{m} \beta_{ij}(y) \frac{\partial}{\partial y_{i}}, \quad \text{for } j = 1, \dots, d,$$
(13)

which map vector-valued functions to vector-valued functions of the same dimension, respectively. More precisely, for any  $\nu \in N$  and a  $\nu$ -dimensional vector-valued function  $\varphi(y) = (\varphi_1(y), \varphi_2(y), \dots, \varphi_\nu(y))^T$ ,

$$(\mathscr{A}_0(\varphi))(y) = ((\mathscr{A}_0(\varphi_1))(y), (\mathscr{A}_0(\varphi_2))(y), \dots, (\mathscr{A}_0(\varphi_\nu))(y))$$

and

$$(\mathscr{A}_{j}(\varphi))(y) = ((\mathscr{A}_{j}(\varphi_{1}))(y), (\mathscr{A}_{j}(\varphi_{2}))(y), \dots, (\mathscr{A}_{j}(\varphi_{\nu}))(y))$$

for j = 1, 2, ..., d.

Moreover, for an index  $\mathbf{i} = (i_1, \dots, i_n) \in \{0, 1, 2, \dots, d\}^n$  and a right-continuous stochastic process  $\{f(t)\}$ , we define an iterated Stratonovich integral with integrand f as

$$J_{\mathbf{i}}[f](t) := \int_{0}^{t} \int_{0}^{t_{1}} \cdots \int_{0}^{t_{n-1}} f(t_{n}) \circ dW_{i_{n}}(t_{n}) \cdots \circ dW_{i_{2}}(t_{2}) \circ dW_{i_{1}}(t_{1}),$$
(14)

which is recursively calculated from inside to outside (see p. 174 of Kloeden and Platen [46]). For ease of exposition, the order of iterated integrations defined in this paper is the reverse of that employed in Kloeden and Platen [46] for any arbitrary index. To lighten notations, for  $f \equiv 1$ , the integrals  $J_i[1](t)$  is abbreviated to  $J_i(t)$ . By convention, we assume  $W_0(t) := t$  and define

$$\|\mathbf{i}\| := \sum_{k=1}^{n} [2 \cdot \mathbf{1}_{\{i_k=0\}} + \mathbf{1}_{\{i_k\neq0\}}]$$
(15)

as a "norm" of the index **i**, which counts k with  $i_k = 0$  twice.

By regarding  $Y^{\epsilon}(1)$  as a function of  $\epsilon$ , it is natural to obtain a path-wise expansion in  $\epsilon$  with random coefficients. According to Watanabe [74], we introduce the following coefficient function  $C_i(y)$  defined by iterative applications of the differential operators (13):

$$C_{\mathbf{i}}(\mathbf{y}) := \mathscr{A}_{i_{\mathbf{i}}}(\dots(\mathscr{A}_{i_{2}}(\boldsymbol{\beta}_{\cdot \mathbf{i}})))\dots)(\mathbf{y}), \tag{16}$$

for an index  $\mathbf{i} = (i_1, \ldots, i_n)$ . Here, for  $i_1 \in \{1, 2, \ldots, d\}$ , the vector  $\beta_{.i_1}(y) = (\beta_{1i_1}(y), \ldots, \beta_{mi_1}(y))^T$  denotes the  $i_1$ th column vector of the dispersion matrix  $\beta(y)$ ; for  $i_1 = 0$ ,  $\beta_{.0}(y)$  refers to the drift vector  $\alpha(y)$  defined in (11). Bypassing the general recursion proposed in Takahashi et al. [66, 67], the nature of the small-time parameterizations in (7) and (10) renders the following simple closed-form expansion with aid of iterated Stratonovich integrals of the type (14) based on Theorem 3.3 in Watanabe [74].

LEMMA 1.  $Y^{\epsilon}(1)$  admits the following path-wise asymptotic expansion

$$Y^{\epsilon}(1) = \sum_{k=0}^{J} Y_k \epsilon^k + \mathcal{O}(\epsilon^{J+1}), \qquad (17)$$

for any  $J \in N$ . Here,  $Y_0 = y_0$  and  $Y_k$  can be written as a closed-form linear combination of iterated Stratonovich integrals, i.e.,

$$Y_{k} = \sum_{\|\mathbf{i}\| = k} C_{\mathbf{i}}(y_{0}) J_{\mathbf{i}}(1),$$
(18)

for k = 1, 2, ..., where the integral  $J_i(1)$ , the norm  $||\mathbf{i}||$ , and coefficient  $C_i(y_0)$  are defined in (14), (15) and (16), respectively.

Indeed, the correction term (18) is obtained from successive applications of the Itô-Stratonovich formula. For any arbitrary dimension r = 1, 2, ..., m, one has the following element-wise form:

$$Y_r^{\epsilon}(1) = \sum_{k=0}^{J} Y_{k,r} \epsilon^k + \mathscr{O}(\epsilon^{J+1}), \quad \text{where } Y_{k,r} = \sum_{\|\mathbf{i}\|=k} C_{\mathbf{i},r}(y_0) J_{\mathbf{i}}(1), \tag{19}$$

with the coefficient

6

 $C_{\mathbf{i},r}(y_0) := \mathscr{A}_{i_n}(\dots(\mathscr{A}_{i_3}(\mathscr{A}_{i_2}(\boldsymbol{\beta}_{ri_1})))\dots)(y_0), \text{ for an index } \mathbf{i} = (i_1,\dots,i_n).$ 

For instance, the first two correction terms are calculated as

$$Y_{1,r} = \sum_{j=1}^{d} \beta_{rj}(y_0) W_j(1) \quad \text{and} \quad Y_{2,r} = \alpha_r(y_0) + \sum_{i_1, i_2=1}^{d} \sum_{l=1}^{m} \beta_{li_2}(y_0) \frac{\partial \beta_{ri_1}}{\partial x_l}(y_0) \int_0^1 \int_0^{t_1} \circ dW_{i_2}(t_2) \circ dW_{i_1}(t_1).$$

We note that the expansion (17) is different from the Wiener chaos decomposition (see, e.g., chapter 1 in Nualart [55]); it can be viewed as a stochastic Stratonovich-Taylor expansion (see, e.g., chapter 6 in Kloeden and Platen [46]) with an arrangement of correction terms according to the power of small-parameter  $\epsilon$ . For ease of exposition, we focus on the derivation of our expansion in this and the next subsection and articulate the theoretical validity of the expansions in the proofs given in Appendix A.

**3.2. Small-time expansion for option valuation: A general framework.** In this section, we seek for a simple closed-form expansion for approximating the price

$$V(0) = E[e^{-rT}p(f(X(T)))] = e^{-rT}E[p(f(X^{\epsilon}(1)))] \equiv e^{-rT}E(Y_1^{\epsilon}(1) - K)^+,$$
(20)

which follows from (4), (5), (7), and (9). To apply the theory of Watanabe [74], we follow the setting in, e.g., Takahashi [61], Kunitomo and Takahashi [48, 49], and Takahashi et al. [67], to consider a standardized random variable

$$Z^{\epsilon} := D(y_0)(Y_1^{\epsilon}(1) - y_0)/\epsilon.$$
<sup>(21)</sup>

By introducing a standard Brownian motion B(t) defined by

$$B(t) = D(y_0) \sum_{j=1}^d \beta_{1j}(y_0) W_j(t), \quad \text{where } D(y) := \left(\sum_{j=1}^d \beta_{1j}^2(y)\right)^{-1/2}, \tag{22}$$

it is easy to see that  $Z^{\epsilon}$  converges to a standard normal random variable B(1) as  $\epsilon \to 0$ . Assuming that  $Z^{\epsilon}$  admits an expansion

$$Z^{\epsilon} = \sum_{k=0}^{J} Z_{k} \epsilon^{k} + \mathcal{O}(\epsilon^{J+1}), \quad \text{for some } J \in N,$$
(23)

the coefficients can be determined by  $Z_i = D(y_0)Y_{i+1,1}$ , for i = 0, 1, 2, ..., where  $Y_{i+1,1}$  are given by (19). Thus, the option price (20) can be expressed as

$$V(0) = \epsilon e^{-rT} D(y_0)^{-1} E(Z^{\epsilon} - z)^+,$$
(24)

where

$$z = D(y_0)(K - y_{01})/\epsilon.$$
 (25)

Thus, our immediate task is to obtain a closed-form expansion for  $E(Z^{\epsilon} - z)^+$ .

Intuitively speaking, based on the expansion for  $Z^{\epsilon}$  given in (23), brute force applications of the classical chain rule to a composition of the generalized function  $T(x) := (x - z)^+$  and  $Z^{\epsilon}$  with the variable  $\epsilon$  yields a Taylor-type expansion for  $(Z^{\epsilon} - z)^+$  as follows:

$$(Z^{\epsilon} - z)^{+} = \sum_{k=0}^{J} \Psi_{k}(z) \epsilon^{k} + \mathscr{O}(\epsilon^{J+1}), \quad \text{for any } J \in N.$$
(26)

Here, the initial term is given by  $\Psi_0(z) = (Z_0 - z)^+$ ; for k = 1, 2, ..., the kth expansion term  $\Psi_k(z)$  is determined by

$$\Psi_k(z) = \sum_{(n,\mathbf{r}(n))\in\mathcal{R}_k} \frac{1}{n!} \frac{\partial^{(n)}T}{\partial x^n} (Z_0) Z_{r_1} Z_{r_2}, \ldots, Z_{r_n},$$

where the index set is defined as

 $\mathcal{R}_k := \{ (n, \mathbf{r}(n)) \mid n = 0, 1, 2, \dots, \mathbf{r}(n) = (r_1, r_2, \dots, r_n) \text{ with } r_i \ge 1 \text{ and } r_1 + r_2 + \dots + r_n = k \}.$ (27)

In particular, the derivatives of T are calculated as

$$\frac{\partial^{(1)}T}{\partial x^1}(x) = 1\{x \ge z\}, \qquad \frac{\partial^{(2)}T}{\partial x^2}(x) = \delta(x-z), \qquad \text{and} \qquad \frac{\partial^{(l)}T}{\partial x^l}(x) = \delta^{(l-2)}(x-z), \quad \text{for } l \ge 3,$$

where  $\delta(x - z)$  is the Dirac delta function centered at z. It is well known that the Dirac delta function  $\delta(x)$  is a generalized function depending on a real variable x such that it is zero for all values of the x except x = 0; and its integral over x from  $-\infty$  to  $\infty$  is equal to one. For many purposes, the Dirac delta can be intuitively manipulated as a function, although it is formally defined as a distribution that is also a measure; see, e.g., Kanwal [42]. Then, by taking expectations on (26), we obtain an expansion

$$E[(Z^{\epsilon} - z)^+] := \sum_{k=0}^{J} \Omega_k(z) \epsilon^k + \mathcal{O}(\epsilon^{J+1}), \quad \text{for any } J \in N,$$
(28)

where the correction term

$$\Omega_k(z) = E\Psi_k(z) \tag{29}$$

will be explicitly determined in what follows.

For k = 0, it is straightforward to deduce the leading term as

$$\Omega_0(z) = E(Z_0 - z)^+ = E(B(1) - z)^+ = \phi(z) - z(1 - N(z)),$$
(30)

where  $\phi(\cdot)$  and  $N(\cdot)$  denote the probability density and cumulative distribution functions of a standard normal variable, respectively. To give a closed-form formula for  $\Omega_k(y)$  with  $k \ge 1$ , we introduce the following two operators. For differentiating a product of an arbitrary function and  $\phi$ , we define a differential operator  $\mathfrak{D}$  such that

$$\mathfrak{D}(f)(x): \frac{\partial f(x)}{\partial x} - xf(x), \quad \text{for any function } f(x). \tag{31}$$

Note that, for any function g(x) and  $\phi(x)$ , the derivative of  $g(x)\phi(x)$  can be simply expressed using (31) as follows:

$$\frac{\partial}{\partial x}[g(x)\phi(x)] = \left[\frac{\partial}{\partial x}g(x) - xg(x)\right]\phi(x) = \mathcal{D}(g)(x)\phi(x).$$

To explicitly express an integration of a product of a polynomial and  $\phi$ , we introduce an integral operator  $\mathcal{I}$  such that, for an arbitrary polynomial  $q(x) := \sum a_n x^n$ ,

$$\mathcal{F}(q)(x) := \int_{x}^{\infty} q(u)\phi(u) \, du \equiv \sum a_{n}q_{n}(x), \tag{32}$$

where the function  $q_n(x) = \int_x^\infty u^n \phi(u) \, du$  is defined in the following lemma.

LEMMA 2. Suppose that  $q_n(x) = \int_x^\infty u^n \phi(u) \, du$ . Thus,  $\{q_n(x): n \ge 0\}$  is a sequence of polynomials recursively determined by

$$q_0(x) = 1 - N(x), \qquad q_1(x) = \phi(x), \qquad q_n(x) = x^{n-1}\phi(x) + (n-1)q_{n-2}(x) \quad \text{for } n = 2, 3, \dots$$
 (33)

**PROOF.** It follows from a straightforward application of the Integration by parts.  $\Box$ 

At the heart of a closed-form formula for the expansion term (29), we introduce conditional expectations of the following type

$$P_{(\mathbf{i}_1,\mathbf{i}_2,\ldots,\mathbf{i}_l)}(z) := E\left(\prod_{w=1}^l J_{\mathbf{i}_w}(1) \,\middle|\, B(1) = z\right) = E\left(\prod_{w=1}^l J_{\mathbf{i}_w}(1) \,\middle|\, \sum_{i=1}^d \lambda_i W_i(1) = z\right),\tag{34}$$

for some indices  $\mathbf{i}_1, \mathbf{i}_2, \dots, \mathbf{i}_l$ , where the constant coefficients are defined by

$$\lambda_i := \beta_{1i}(y_0) \left( \sum_{k=1}^d \beta_{1k}^2(y_0) \right)^{-1/2}, \quad \text{for } i = 1, 2, \dots, d.$$
(35)

Starting from Itô [39], investigation of iterated stochastic integrals has become an important and challenging issue in probablity and stochastic modeling; see, e.g., Kloeden and Platen [46], Houdre and Perez-Abreu [37], Peccati and Taqqu [58], and the references therein. As an important building block for constructing small-diffusion type expansions, conditional expectation involving iterated Itô integrals can be found in, e.g., Yoshida [76], Takahashi [61, 62, 63], Kunitomo and Takahashi [48, 49], Takahashi and Yamada [70], Takahashi et al. [66, 67], Kawai [45], Jaeckel and Kawai [40], and Gobet et al. [30, 31]. Compared with the conditional expectations needed for small-diffusion expansions, (34) is irrelevant of the complexity of the functional form of the drift and diffusion. However, since the large-deviation based expansion for heat-kernel discussed in Watanabe [74], seeking for algorithms and formulas for calculating conditional expectations involving iterated Stratonovich integrals in closed form has become an open problem. In §4, we will provide an efficient algorithm for calculating (34) as a multivariate polynomial in *z*, which will substantially enhance the feasibility of calculating high-order expansions.

In the following proposition, we express any arbitrary correction term  $\Omega_k(z)$  with  $k \ge 1$  by a simple closed-form formula, which can be regarded as an explicit solution to the recursion-based general scheme proposed in Takahashi et al. [66, 67].

**PROPOSITION 1.** For any  $k \in N$ , the kth order correction term  $\Omega_k(z)$  admits the following explicit representation

$$\Omega_{k}(z) = D(y_{0}) \sum_{\|\mathbf{i}\| = k+1}^{n} C_{\mathbf{i},1}(y_{0}) \mathcal{I}(P_{(\mathbf{i})})(z)$$
  
+ 
$$\sum_{\substack{n \ge 2, \\ (n, \mathbf{r}(n)) \in \mathcal{R}_{k}}}^{n \ge 2,} \frac{(-1)^{n-2}}{n!} D(y_{0})^{n} \sum_{\substack{\|\mathbf{i}_{w}\| = r_{w}+1, \\ w=1,2,\dots,n}}^{n} \left(\prod_{w=1}^{n} C_{\mathbf{i}_{w},1}(y_{0})\right) \mathfrak{D}^{n-2}(P_{(\mathbf{i}_{1},\mathbf{i}_{2},\dots,\mathbf{i}_{n})})(z)\phi(z),$$
(36)

where  $D(y_0)$ ,  $\|\cdot\|$ ,  $C_{\mathbf{i}_w,1}(y_0)$ ,  $\mathcal{I}$ ,  $P_{(\mathbf{i}_1,\mathbf{i}_2,\ldots,\mathbf{i}_n)}$ ,  $\mathcal{R}_k$ , and  $\mathcal{D}$  are defined in (22), (15), (16), (32), (34), (27), and (31), respectively.

PROOF. See Appendix A.

Without loss of generality, we exemplify the first three closed-form correction terms as follows:

$$\Omega_{1}(z) = D(y_{0}) \sum_{\|\mathbf{i}\|=2} C_{\mathbf{i},1}(y_{0}) \mathcal{I}(P_{(\mathbf{i})})(z),$$
(37)

$$\Omega_{2}(z) = D(y_{0}) \sum_{\|\mathbf{i}\|=3} C_{\mathbf{i},1}(y_{0}) \mathcal{I}(P_{(\mathbf{i})})(z) + \frac{D(y_{0})^{2}}{2} \sum_{\|\mathbf{i}_{1}\|=\|\mathbf{i}_{2}\|=2} C_{\mathbf{i}_{1},1}(y_{0}) C_{\mathbf{i}_{2},1}(y_{0}) P_{(\mathbf{i}_{1},\mathbf{i}_{2})}(z) \phi(z),$$
(38)

$$\Omega_{3}(z) = D(y_{0}) \sum_{\|\mathbf{i}\|=4} C_{\mathbf{i},1}(y_{0}) \mathcal{F}(P_{(\mathbf{i})})(z) + D(y_{0})^{2} \sum_{\|\mathbf{i}_{1}\|=2, \|\mathbf{i}_{2}\|=3} C_{\mathbf{i}_{1},1}(y_{0}) C_{\mathbf{i}_{2},1}(y_{0}) P_{(\mathbf{i}_{1},\mathbf{i}_{2})}(z) \phi(z) - \frac{D(y_{0})^{3}}{6} \sum_{\|\mathbf{i}_{1}\|=\|\mathbf{i}_{2}\|=\|\mathbf{i}_{3}\|=2} C_{\mathbf{i}_{1},1}(y_{0}) C_{\mathbf{i}_{2},1}(y_{0}) C_{\mathbf{i}_{3},1}(y_{0}) \mathcal{D}(P_{(\mathbf{i}_{1},\mathbf{i}_{2},\mathbf{i}_{3})})(z) \phi(z),$$
(39)

where the coefficients are explicitly given by

$$C_{(i_1),1} = \beta_{1i_1}(y_0),$$
  
$$C_{(i_1,i_2),1} = \sum_{i=1}^m \beta_{ii_2}(y_0) \frac{\partial}{\partial x_i} \beta_{1i_1}(y_0),$$

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$$C_{(i_{1}, i_{2}, i_{3}), 1} = \sum_{j=1}^{m} \beta_{ji_{3}}(y_{0}) \frac{\partial}{\partial x_{j}} \left( \sum_{i=1}^{m} \beta_{ii_{2}}(y_{0}) \frac{\partial}{\partial x_{i}} \beta_{1i_{1}}(y_{0}) \right),$$
  
$$C_{(i_{1}, i_{2}, i_{3}, i_{4}), 1} = \sum_{k=1}^{m} \beta_{ki_{4}}(y_{0}) \frac{\partial}{\partial x_{k}} \left( \sum_{j=1}^{m} \beta_{ji_{3}}(y_{0}) \frac{\partial}{\partial x_{j}} \left( \sum_{i=1}^{m} \beta_{ii_{2}}(y_{0}) \frac{\partial}{\partial x_{i}} \beta_{1i_{1}}(y_{0}) \right) \right).$$

Finally, by plugging (25) into (28) and recalling (24) with  $\epsilon = \sqrt{T}$ , a *J*th order expansion approximation for the option price (20) is defined by

$$V^{(J)}(0) := \sqrt{T} e^{-rT} D(y_0)^{-1} \sum_{k=0}^{J} \Omega_k(D(y_0)(K - y_{01})/\sqrt{T}) T^{k/2},$$
(40)

where  $y_0 = (f(x_{01}, x_{02}, \dots, x_{0m}), x_{02}, \dots, x_{0m})$ . Thus, the following proposition states the validity of the expansion (40) under the technical assumptions introduced in §2.

PROPOSITION 2. Under the technical Assumptions 1, 2, and 3, we have

$$\sup_{(x>0, x_0\in\mathcal{S}, \theta\in\Theta)} |V(0) - V^{(J)}(0)| \le cT^{(J+1)/2},\tag{41}$$

for any  $J \in N$  and some constant c > 0, where S is any compact subset of E (the state space of the diffusion X).

PROOF. See Appendix A.

Before moving to the next section, we remark that the error estimate in (41) is analogous to the characterization of a remainder term of Taylor expansion for smooth functions in classical calculus. Similar to the theory of Taylor expansion, such an error estimate is a local property. However, as demonstrated through the computational results in §5.1, the accuracy of expansions is not restricted to small values of *T*; instead, the performance can be enhanced by increasing the number of correction terms.

**4. Explicit calculation of conditional expectation (34).** In this section, we dwell on a general and efficient algorithm for explicitly calculating conditional expectation (34), which is different from the existing results on iterated Itô integrals; see, e.g., Yoshida [76], Takahashi [61, 62, 63], Kunitomo and Takahashi [48, 49], Takahashi and Yamada [70], Takahashi et al. [66, 67], Kawai [45], Jaeckel and Kawai [40], and Gobet et al. [30, 31]. To introduce a fundamental tool for circumventing the challenge in calculating (34), we generalize (34) to the following form:

$$Q_{(\mathbf{i}_1,\mathbf{i}_2,\ldots,\mathbf{i}_l)}(\mathbf{x}) := E\left(\prod_{w=1}^l J_{\mathbf{i}_w}(1) \middle| W(1) = \mathbf{x}\right), \quad \text{for } \mathbf{x} \in \mathbb{R}^d,$$
(42)

where the conditioning is strengthened to the multidimensional Brownian motion. Such an extension will be potentially useful in a wide range of studies in theoretical and applied probability as well as stochastic modeling.

**4.1. From one-dimensional to multidimensional conditioning.** We begin with clarifying how the conditional expectation (34) can be calculated based on (42). For the coefficients (35), we assume  $\lambda_1 \neq 0$  without loss of generality. It follows from (34) that

$$P_{(\mathbf{i}_{1},\mathbf{i}_{2},\ldots,\mathbf{i}_{l})}(z) = \int_{(z_{2},\ldots,z_{m})\in\mathbb{R}^{m-1}} E\left(\prod_{w=1}^{l} J_{\mathbf{i}_{w}}(1) \left| \sum_{i=1}^{d} \lambda_{i} W_{i}(1) = z, W_{2}(1) = z_{2}\ldots, W_{d}(1) = z_{d} \right) \times \varphi(z_{2}, z_{3},\ldots,z_{d} \mid z) \, dz_{2}\ldots dz_{d},$$
(43)

where  $\varphi(z_2, z_3, \dots, z_d | z)$  denotes the density of the following conditional distribution:

$$(W_2(1), W_3(1), \dots, W_d(1))$$
 given  $\sum_{i=1}^d \lambda_i W_i(1) = z.$  (44)

It is straightforward to observe that the conditional law of (44) follows a normal distribution with a mean vector  $(\lambda_2, \lambda_3, \ldots, \lambda_d)^T z$  and a covariance matrix

$$\Sigma := (\Sigma_{ij})_{(d-1)\times(d-1)} = \begin{pmatrix} 1 - \lambda_2^2 & -\lambda_2\lambda_3 & \cdots & -\lambda_2\lambda_d \\ -\lambda_3\lambda_2 & 1 - \lambda_3^2 & \cdots & -\lambda_3\lambda_d \\ \vdots & \vdots & \ddots & \vdots \\ -\lambda_d\lambda_2 & -\lambda_d\lambda_3 & \cdots & 1 - \lambda_d^2 \end{pmatrix}.$$

Thus, its moment generating function can be explicitly given by

$$\psi(\vartheta_1, \vartheta_2, \dots, \vartheta_{d-1}) := E \left[ \exp\left(\sum_{k=1}^{d-1} \vartheta_k W_k(1)\right) \middle| \sum_{i=1}^d \lambda_i W_i(1) = z \right]$$
$$= \exp\left(\sum_{k=1}^{d-1} \vartheta_k \lambda_{k+1} z + \frac{1}{2} \sum_{i, j=1}^d \vartheta_i \vartheta_j \Sigma_{ij} \right).$$
(45)

On the other hand, for a vector  $\mathbf{z} := (z, z_2, ..., z_d)$ , the conditional expectation in the integrand of (43) satisfies

$$E\left(\prod_{w=1}^{l} J_{\mathbf{i}_{w}}(1) \left| \sum_{i=1}^{d} \lambda_{i} W_{i}(1) = z, W_{2}(1) = z_{2}, \dots, W_{d}(1) = z_{d} \right.\right) = E\left(\prod_{w=1}^{l} J_{\mathbf{i}_{w}}(1) \left| W(1) = \Lambda^{-1} \mathbf{z} \right.\right),$$

where the matrix  $\Lambda$  is defined by

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$$\Lambda := \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_d \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}.$$

Provided that the conditional expectation (42) can be calculated as a multivariate polynomial in x, we assume

$$Q_{(\mathbf{i}_1,\mathbf{i}_2,\ldots,\mathbf{i}_l)}(\Lambda^{-1}\mathbf{z}) \equiv E\left(\prod_{w=1}^l J_{\mathbf{i}_w}(1) \,\middle|\, W(1) = \Lambda^{-1}\mathbf{z}\right) = \sum_{n_1,n_2,\ldots,n_d \in N} c(n_1, n_2, \ldots, n_d) z^{n_1} z_2^{n_2} \ldots z_d^{n_d},$$

where  $c(n_1, n_2, ..., n_d)$  is the coefficient corresponding to the term  $z^{n_1} z_2^{n_2} ... z_d^{n_d}$ . Thus, it follows from (43) that

$$P_{(\mathbf{i}_1,\mathbf{i}_2,\ldots,\mathbf{i}_l)}(z_1) = \sum_{\substack{n_1,n_2,\ldots,n_d \in N}} c(n_1,n_2,\ldots,n_d) z^{n_1} \int_{(z_2,\ldots,z_m) \in \mathbb{R}^{m-1}} z_2^{n_2} \ldots z_d^{n_d} \varphi(z_2,z_3,\ldots,z_d \mid z) \, dz_2 \ldots dz_d$$
$$= \sum_{\substack{n_1,n_2,\ldots,n_d \in N}} c(n_1,n_2,\ldots,n_d) z^{n_1} M(n_2,\ldots,n_d),$$

where  $M(n_2, \ldots, n_d)$  is a cross moment defined by

$$M(n_2, \dots, n_d) := E\left(W_2(1)^{n_2} W_3(1)^{n_3} \dots W_d^{n_d}(1) \left| \sum_{i=1}^d \lambda_i W_i(1) = z \right).$$
(46)

We note that a closed-form expression for (46) can be obtained from differentiating the moment generating function (45), i.e.,

$$M(n_2,\ldots,n_d) = \frac{\partial^{n_2+\cdots+n_d}\psi(\vartheta_1,\vartheta_2,\ldots,\vartheta_{d-1})}{\partial\vartheta_1^{n_2}\partial\vartheta_2^{n_3}\ldots\partial\vartheta_{d-1}^{n_d}}\bigg|_{\vartheta_1=\vartheta_2=\cdots=\vartheta_{d-1}=0}$$

**4.2.** Calculation of (42). For any arbitrary indices  $\mathbf{i}_1, \mathbf{i}_2, \dots, \mathbf{i}_l$ , we propose a general method for calculating the conditional expectation (42). In the construction of diagonal expansion for heat kernel, Watanabe [74] outlined the challenges in computing conditional expectation of the type (42). By discretizing stochastic integrals, Uemura [73] showed that (42) has the structure of a polynomial in  $\mathbf{x} = (x_1, x_2, \dots, x_m)$  with some unknown coefficients.

In addition to the iterated Stratonovich integral defined in (14), let

$$I_{\mathbf{i}}[f](t) := \int_{0}^{t} \int_{0}^{t_{1}} \cdots \int_{0}^{t_{n-1}} f(t_{n}) \, dW_{i_{n}}(t_{n}) \cdots \, dW_{i_{2}}(t_{2}) \, dW_{i_{1}}(t_{1}) \tag{47}$$

be an iterated Itô integral with the right-continuous integrand f for an index  $\mathbf{i} = (i_1, \dots, i_n) \in \{0, 1, 2, \dots, d\}^n$ . To lighten the notation, for  $f \equiv 1$ , the integral  $I_i[1](t)$  is abbreviated as  $I_i(t)$ . Before discussing details, we outline a brief description of a general algorithm for explicitly computing any arbitrary conditional expectation of the type (42). It is noteworthy that this algorithm can be conveniently implemented using any symbolic

package, e.g., Mathematica. In what follows, the iterated Itô integrals may involve not only stochastic integrals with respect to Brownian motions in the Itô sense but also Lebesgue integrals with respect to time variables.

#### Algorithm 1

• Convert multiplication of Stratonovich integrals to a linear combination of iterated Stratonovich integrals.

- Convert each iterated Stratonovich integral to a linear combination of iterated Itô integrals.
- Compute conditional expectation for each iterated Itô integrals.

**4.2.1.** Conversion from multiplications of Stratonovich integrals to linear combinations. In this subsection, we provide a simple recursive algorithm for converting any arbitrary multiplication of iterated Stratonovich integrals to a linear combination. Let -i and i – denote the index obtained by deleting the first and the last components of an arbitrary index i, respectively. According to Tocino [71], for a product of two iterated Stratonovich integrals as defined in (14), it follows that

$$J_{\alpha}(t)J_{\beta}(t) = \int_{0}^{t} J_{\alpha}(s)J_{-\beta}(s) \circ dW_{\beta_{1}}(s) + \int_{0}^{t} J_{-\alpha}(s)J_{\beta}(s) \circ dW_{\alpha_{1}}(s),$$
(48)

for any arbitrary indices  $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_p)$  and  $\boldsymbol{\beta} = (\beta_1, \beta_2, \dots, \beta_q)$ . Iterative applications of this relation render a linear combination form of  $J_{\boldsymbol{\alpha}}(t)J_{\boldsymbol{\beta}}(t)$ . For example, let  $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$  and  $\boldsymbol{\beta} = (\beta_1, \beta_2)$ , iterative applications of (48) yield a linear combination form of  $J_{\boldsymbol{\alpha}}(1)J_{\boldsymbol{\beta}}(1)$  as

$$J_{\alpha}(1)J_{\beta}(1) = J_{(\alpha_{1},\alpha_{2},\beta_{1},\beta_{2},\alpha_{3})}(1) + J_{(\alpha_{1},\beta_{1},\beta_{2},\alpha_{2},\alpha_{3})}(1) + J_{(\beta_{1},\beta_{2},\alpha_{1},\alpha_{2},\alpha_{3})}(1) + J_{(\beta_{1},\alpha_{1},\beta_{2},\alpha_{2},\alpha_{3})}(1) + J_{(\beta_{1},\alpha_{1},\alpha_{2},\beta_{2},\alpha_{3})}(1) + J_{(\alpha_{1},\alpha_{2},\beta_{2},\alpha_{3})}(1) + J_{(\alpha_{1},\alpha_{2},\alpha_{3},\beta_{1},\beta_{2})}(1) + J_{(\alpha_{1},\alpha_{2},\beta_{1},\alpha_{3},\beta_{2})}(1) + J_{(\alpha_{1},\alpha_{2},\alpha_{3},\beta_{2})}(1) + J_{(\alpha_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{2})}(1) + J_{(\alpha_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{2})}(1) + J_{(\alpha_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{2})}(1) + J_{(\alpha_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{2},\alpha_{3},\beta_{3},\beta_{3},\alpha_{3},\beta_$$

Thus, iterated applications of the above algorithm yield a conversion from a multiplication of any number of iterated Stratonovich integrals to a linear combination. Therefore, our immediate task is reduced to the calculation of conditional expectation of iterated Stratonovich integrals.

**4.2.2.** Conversion from iterated Stratonovich integrals to Itô integrals. In this subsection, we briefly adapt an algorithm proposed in Kloeden and Platen [46] for systematically converting an arbitrary iterated Stratonovich integral to a linear combination of iterated Itô Integrals. For the index  $\mathbf{i} = (i_1, \ldots, i_n) \in \{0, 1, 2, \ldots, d\}^n$ , its length is defined by  $l(\mathbf{i}) := l((i_1, \ldots, i_n)) = n$ . Let  $\nu$  denote the index with zero length, i.e.,  $l(\nu) = 0$ . We also recall that  $W_0(t) := t$ . According to p. 172 of Kloeden and Platen [46], the conversion between iterated Stratonovich integrals defined in (14) and iterated Itô integrals defined in (47) can be achieved via a recursive algorithm. For the case of  $l(\mathbf{i}) = 0$  or 1, it is easy to have  $J_{\mathbf{i}}(t) = I_{\mathbf{i}}(t)$ ; for the case of  $l(\mathbf{i}) \ge 2$ , a general conversion scheme can be implemented via an iteration:

$$J_{\mathbf{i}}(t) = I_{(i_1)}[J_{-\mathbf{i}}(\cdot)](t) + \mathbb{1}_{\{i_1 = i_2 \neq 0\}} I_{(0)}[\frac{1}{2}J_{-(-\mathbf{i})}(\cdot)](t).$$
(49)

For instance, if  $l(\mathbf{i}) = 2$ , we have

$$J_{\mathbf{i}}(t) = I_{\mathbf{i}}(t) + \frac{1}{2} \mathbf{1}_{\{i_1 = i_2 \neq 0\}} I_{(0)}(t).$$

More explicitly, the conversion of Stratonovich integral  $J_{(i_1, i_2)}(1)$ , for  $i_1, i_2 \in \{1, 2, ..., d\}$ , yields that

$$\int_0^1 \int_0^{t_1} 1 \circ dW_{i_2}(t_2) \circ dW_{i_1}(t_1) = \int_0^1 W_{i_2}(t_1) \circ dW_{i_1}(t_1) = \int_0^1 W_{i_2}(t_1) dW_{i_1}(t_1)$$

for  $i_1 \neq i_2$ ;

$$\int_0^1 \int_0^{t_1} 1 \circ dW_{i_2}(t_2) \circ dW_{i_1}(t_1) = \int_0^1 W_{i_1}(t_1) dW_{i_1}(t_1) + \frac{1}{2} = \frac{1}{2} W_{i_1}(1)^2,$$

for  $i_1 = i_2$ .

Now, with the conversion algorithm (49), we are able to express any arbitrary iterated Stratonovich integral (in the linear combination converted from the multiplication  $\prod_{w=1}^{l} J_{i_w}(1)$ ) as a linear combination of iterated Itô integrals. Thus, our immediate task becomes the calculation of conditional expectation of iterated Itô integrals, which will be intensively discussed in the following subsection.

**4.2.3.** A closed-form formula for conditional expectation of iterated Itô integrals. As the most challenging issue for completing our closed-form expansion, we propose a novel formula for calculating conditional expectation of the following general form:

$$E[I_{\mathbf{i}}(1) | W(1) = \mathbf{x}] = E\left(\int_{0}^{1} \int_{0}^{t_{1}} \cdots \int_{0}^{t_{n-1}} dW_{i_{n}}(t_{n}) \cdots dW_{i_{2}}(t_{2}) dW_{i_{1}}(t_{1}) \middle| W(1) = \mathbf{x}\right),$$
(50)

for any arbitrary index  $\mathbf{i} = (i_1, i_2, ..., i_n) \in \{0, 1, 2, ..., d\}^n$  and vector  $\mathbf{x} = (x_1, x_2, ..., x_d)$ .

Our formula for the conditional expectation (50) is different from the existing results. For one-dimensional Brownian motion, an explicit formula for conditional expectation of multiple Itô integrals with deterministic integrands and without Lebesgue integrals on the time variable was introduced in Nualart et al. [56] via Wiener-chaos decomposition; see, e.g., chapter 1 in Nualart [55]. Takahashi et al. [66] adapted this result to the case with iterated Itô integrals. To implement small-diffusion type asymptotic expansions, such a formula was applied and generalized in order to incorporate multidimensional Brownian motions in, e.g., Yoshida [76, 77], Takahashi [61, 62, 63], Kunitomo and Takahashi [48, 49], Takahashi et al. [66, 67], and Shiraya et al. [60]. By converting conditional expectations to unconditional ones via Hermite polynomials, an alternative ordinary-differential-equation-based scheme for computing conditional expectations can be found in Takahashi et al. [66, 67], and Takahashi and Toda [68].

**PROPOSITION 3.** For any arbitrary index  $\mathbf{i} = (i_1, i_2, \dots, i_n)$  with  $i_1, i_2, \dots, i_n \in \{0, 1, \dots, d\}$ , we have

$$E[I_{\mathbf{i}}(1) | W(1) = \mathbf{x}] = \frac{1}{n!} \sum_{k_1=0}^{n_{\mathbf{i}}(1)} \cdots \sum_{k_d=0}^{n_{\mathbf{i}}(d)} (-1)^{\sum_{l=1}^{d} (n_{\mathbf{i}}(l)-k_l)/2} \prod_{l=1}^{d} \left[ \nu(n_{\mathbf{i}}(l)-k_l) \binom{n_{\mathbf{i}}(l)}{k_l} \right] x_1^{k_1}, \dots, x_d^{k_d},$$
(51)

where  $n_i(l)$  denotes the total number of l's appearing in **i**; the function  $\nu$  is defined by

$$\nu(n) = \prod_{k=0}^{(n/2)-1} {\binom{n-2k}{2}} / {\binom{n}{2}}!,$$

if n is an even integer, and 0 otherwise.

PROOF. See Appendix B.

In particular, for d = 1, 2, we illustrate the formula (51) via the following two examples. For d = 1 and  $i_1, i_2, \ldots, i_n \in \{0, 1\}$ , we have

$$E[I_{\mathbf{i}}(1) | W(1) = x] = \sum_{k_1=0}^{n_{\mathbf{i}}(1)} \frac{1}{n!} (-1)^{(n_{\mathbf{i}}(1)-k_1)/2} \nu(n_{\mathbf{i}}(1)-k_1) \binom{n_{\mathbf{i}}(1)}{k_1} x^{k_1}.$$

For d = 2 and  $i_1, i_2, \ldots, i_n \in \{0, 1, 2\}$ , we have

$$E[I_{\mathbf{i}}(1) | W(1) = \mathbf{x}] = \sum_{k_2=0}^{n_{\mathbf{i}}(2)} \sum_{k_1=0}^{n_{\mathbf{i}}(1)} \frac{1}{n!} (-1)^{(n_{\mathbf{i}}(1)+n_{\mathbf{i}}(2)-k_1-k_2)/2} \nu(n_{\mathbf{i}}(2)-k_2) \nu(n_{\mathbf{i}}(1)-k_1) \binom{n_{\mathbf{i}}(1)}{k_1} \binom{n_{\mathbf{i}}(2)}{k_2} x_1^{k_1} x_2^{k_2}.$$

**5. Examples and computational results.** To demonstrate the numerical performance of our method, this section is devoted to examples and computational results. In §5.1, we employ the valuation of European options under various constant elasticity of variance type models (see Cox [16]) to illustrate the efficiency of our expansion. In §5.2, we apply our expansion to the valuation of options on VIX, which is a challenging issue in financial engineering because of the complexity of VIX dynamics implied by that of the stochastic variance. Without loss of generality, we employ the GARCH diffusion (see, e.g., Christoffersen et al. [14]) and its multifactor generalization to the Gatheral double lognormal stochastic volatility (hereafter DLN-SV) model (see, e.g., Gatheral [27]) as two examples to illustrate the applicability of our method to analytically intractable non-Lévy and non-affine models.

In each example, we begin by systematically nesting the specific model into the general framework proposed in §2 in order to symbolically implement the closed-form expansion via the general formulas (40) and (36). To limit the length of the paper, we will not include the closed-form expansion formulas, which will be provided in the form of Mathematica notebook upon request. The symbolic computation of asymptotic expansions are implemented in Mathematica; the numerical valuation of the benchmark values (including analytical pricing formulas for CEV type models and Monte Carlo simulations for the GARCH diffusion and DLN-SV models) are programmed in MATLAB. All the numerical experiments are conducted on a laptop PC with an Intel(R) Pentium(R) M 1.73 GHz processor and 2 GB of RAM running Windows XP Professional.

**5.1. Illustrations from valuation of European options under CEV type models.** The CEV type models offer a simple but flexible method for capturing the randomness in volatility, the leverage effect, and even credit risk; see, e.g., Cox [16], Davydov and Linetsky [19], Andersen and Brotherton-Ratcliffe [3], as well as Carr and Linetsky [10]. We assume that the risk-neutral dynamics of an underlying asset is given by the following SDE:

$$dS(t) = rS(t) dt + \delta S(t)^{\beta+1} dW(t), \qquad S(0) = s_0 > 0,$$
(52)

for some constants r,  $\delta$ , and  $\beta$ . By flexible choices of  $\beta$ , which controls the relation between the underlying price and its volatility, the specification of (52) nests a number of celebrated models, e.g., the Black-Scholes model obtained from  $\beta = 0$  (see Black and Scholes [6] and Merton [53]), the Cox-Ingersoll-Ross (CIR) model obtained from  $\beta = -1/2$  (see Cox et al. [17]), and the absolute process obtained from  $\beta = -1$  (see Cox [16] and Davydov and Linetsky [19]). Various alternative methods for approximating option price and implied volatility under the CEV type (or even more general local volatility) models can be found in, e.g., Hagan and Woodward [34], chapter 10 of Lipton [50], chapter 5 of Henry-Labordère [35], Gobet et al. [30], and Gatheral et al. [28].

Based on the analytical tractability of CEV type models, we employ the closed-form formulas for option valuation (see, e.g., Cox [16], Schroder [59], and Davydov and Linetsky [19]) to generate benchmark true values and thus numerically validate our expansions. According to the setting given in (3), it is straightforward to obtain closed-form expansions via (36) and (40). In Table 1, we report the computational results for comparing the fourth and eighth order expansions with the benchmark true values for the maturities T = 1 and 2 and the strikes K = 80, 90, 100, 110, and 120 for four choices of  $\beta$ , i.e.,  $\beta = 0$ , -1/4, -1/2, and -1. The asymptotic refers to the expansion approximations. The error is calculated by the difference between the expansion and the true value. It is evident that the accuracy of the expansions can be obtained at a relatively small order (the fourth in this case) and improved as the order increases. To further demonstrate the performance and robustness of our expansion, we plot the uniform absolute errors for a relatively wide range of strikes  $K \in \{80, 81, \ldots, 120\}$  and for maturities T = 1 and 2 in Figure 1. The Jth order uniform error is calculated from

$$e^{(J)} := \max_{K \in \{80, 81, \dots, 120\}} |V(0) - V^{(J)}(0)|.$$

As seen from Figure 1, the increase of orders results in the decrease of uniform errors. This suggests that better numerical accuracy can be attained by higher order expansions, which will become increasingly feasible to obtain because of rapid improvement in computing technology. We note that Assumption 2 is violated for some model specifications ( $\beta = -1/4$  and -1/2). However, the computational results suggest the wide applicability of our expansion method beyond the theoretical assumptions.

Moreover, in Figure 2, we demonstrate the efficiency of our method by comparing the average uniform absolute error for pricing options with maturity T = 1 over the strikes from  $\{80, 81, \ldots, 120\}$  and the corresponding computing time with those resulting from Monte Carlo simulation methods. For simulations, on the one hand, we employ an exact simulation method by sampling the noncentral chi-square distributions; see, e.g., chapter 3 in Glasserman [29]; on the other hand, we employ the Euler discretization; see, e.g., chapter 6 in Glasserman [29]. Note that the latter strategy sheds light on the cases where exact simulation is impractical or impossible and discretization is inevitable. The comparisons suggest that our expansions significantly outperform both of these two commonly used Monte Carlo simulation methods.

Before closing this section, we compare the performance of our expansion with those of Hagan and Woodward [34], Henry-Labordère [35], Gobet et al. [30], and Gatheral et al. [28]. In Table 2, we report what orders in our expansion are required to obtain comparable accuracy in terms of the Black-Scholes implied volatility. For our expansion, the error in implied volatility is calculated from the difference between the implied volatility of our expansion value and that of the benchmark value given by the closed-form formula; see, e.g., Cox [16] and Schroder [59]. For the alternative methods, the error is calculated from the difference between the implied volatility expansion and the implied volatility of the benchmark value. The errors of the two selected (the second and the fourth) orders of our expansion either sandwich or exhibit magnitudes similar to those of the aforementioned alternative methods (with negligible differences).

**5.2.** Applications in valuation of options on VIX. VIX (the S&P500 implied volatility index; see CBOE [12]) measures market expectations of near term (next 30 calendar days) volatility conveyed by index option prices. Since volatility often signifies financial turmoil, VIX is often referred to as the "investor fear gauge." Options on VIX have become major risk management tools. As important hedging instruments, call options on VIX are often used to manage downside risk. In particular, through rolling options on VIX with one-month maturity, VXTH (the VIX tail hedge; see CBOE [13]) proposed by CBOE has shown its indispensable role as a powerful hedging tool for protecting portfolios against tail risk. In this section, we apply our asymptotic expansion method to the valuation of options on VIX.

Parameters T K		Benchmark	4th order	expansion	8th order expansion		
		True value	Asymptotic	Error	Asymptotic Er		
			$\beta = 0$				
1	80	24.14718964	24.14693216	$2.57 \times 10^{-4}$	24.14718963	$1.25 \times 10^{-8}$	
	90	16.97187578	16.97163582	$2.40 \times 10^{-4}$	16.97187577	$1.06 \times 10^{-8}$	
	100	11.34847683	11.34823719	$2.40 \times 10^{-4}$	11.34847681	$1.06 \times 10^{-8}$	
	110	7.25577635	7.25553699	$2.40 \times 10^{-4}$	7.25577634	$1.06 \times 10^{-8}$	
	120	4.46330171	4.46307640	$2.25 \times 10^{-4}$	4.46330170	$8.89 \times 10^{-9}$	
2	80	28.30846514	28.30650378	$1.96 \times 10^{-3}$	28.30846479	$3.49 \times 10^{-7}$	
	90	21.95705499	21.95511675	$1.94 \times 10^{-3}$	21.95705465	$3.40 \times 10^{-7}$	
	100	16.72842463	16.72648665	$1.94 \times 10^{-3}$	16.72842430	$3.40 \times 10^{-7}$	
	110	12.55715618	12.55521841	$1.94 \times 10^{-3}$	12.557155840	$3.40 \times 10^{-7}$	
	120	9.31369441	9.31177426	$1.92 \times 10^{-3}$	9.31369407	$3.33 \times 10^{-7}$	
			$\beta = -1/4$				
1	80	24.29700872	24.29676550	$2.43 \times 10^{-4}$	24.29700871	$1.08 \times 10^{-8}$	
	90	17.07894600	17.07870793	$2.38 \times 10^{-4}$	17.07894599	$1.06 \times 10^{-8}$	
	100	11.35005220	11.34981264	$2.40 \times 10^{-4}$	11.35005219	$1.06 \times 10^{-8}$	
	110	7.14025331	7.14001225	$2.41 \times 10^{-4}$	7.14025330	$1.06 \times 10^{-8}$	
	120	4.26509695	4.26485927	$2.38 \times 10^{-4}$	4.26509694	$1.02 \times 10^{-8}$	
2	80	28.55925556	28.55733393	$1.92 \times 10^{-3}$	28.55925521	$3.54 \times 10^{-7}$	
	90	22.11232682	22.11039699	$1.93 \times 10^{-3}$	22.11232648	$3.40 \times 10^{-7}$	
	100	16.73274849	16.73081135	$1.94 \times 10^{-3}$	16.73274815	$3.40 \times 10^{-7}$	
	110	12.39509455	12.39315000	$1.95 \times 10^{-3}$	12.39509421	$3.39 \times 10^{-7}$	
	120	9.00454690	9.00259377	$1.95  imes 10^{-3}$	9.00454669	$3.06 \times 10^{-7}$	
			$\beta = -1/2$				
1	80	24.45553812	24.45533260	$2.06 \times 10^{-4}$	24.45553812	$4.97 \times 10^{-9}$	
	90	17.19001023	17.18978314	$2.27 \times 10^{-4}$	17.19001022	$7.42 \times 10^{-9}$	
	100	11.35480260	11.35456392	$2.39 \times 10^{-4}$	11.35480259	$1.01 \times 10^{-8}$	
	110	7.02893190	7.02868214	$2.50  imes 10^{-4}$	7.02893189	$1.24 \times 10^{-8}$	
	120	4.07439179	4.07412303	$2.69 \times 10^{-4}$	4.07439177	$2.08 \times 10^{-8}$	
2	80	28.82489615	28.82312246	$1.77 \times 10^{-3}$	28.82489602	$1.34 \times 10^{-7}$	
	90	22.27702410	22.27515601	$1.87 \times 10^{-3}$	22.27702383	$2.66 \times 10^{-7}$	
	100	16.74584949	16.74392228	$1.93 \times 10^{-3}$	16.74584917	$3.20 \times 10^{-7}$	
	110	12.24351006	12.24152619	$1.98 \times 10^{-3}$	12.24350970	$3.64 \times 10^{-7}$	
	120	8.70980382	8.70773767	$2.07 \times 10^{-3}$	8.70980337	$4.47 \times 10^{-7}$	
			$\beta = -1$				
1	80	24.80176688	24.80158145	$1.86 \times 10^{-4}$	24.80176686	$1.72 \times 10^{-8}$	
	90	17.42594029	17.42571707	$2.23 \times 10^{-4}$	17.42594028	$1.21 \times 10^{-8}$	
	100	11.37418604	11.37394286	$2.43 \times 10^{-4}$	11.37418603	$1.07 \times 10^{-8}$	
	110	6.81790584	6.81764162	$2.64 \times 10^{-4}$	6.81790583	$9.33 \times 10^{-9}$	
	120	3.71352164	3.71321232	$3.09 \times 10^{-4}$	3.71352164	$3.53 \times 10^{-9}$	
2	80	29.41089763	29.40917823	$1.72 \times 10^{-3}$	29.41089821	$5.83 \times 10^{-7}$	
	90	22.64091260	22.63903080	$1.88 \times 10^{-3}$	22.64091245	$1.51 \times 10^{-7}$	
	100	16.80039525	16.79841820	$1.98 \times 10^{-3}$	16.80039494	$3.02 \times 10^{-7}$	
	110	11.96994656	11.96787000	$2.08 \times 10^{-3}$	11.96994625	$3.15 \times 10^{-7}$	
	120	8.15849610	8.15623031	$2.27 \times 10^{-3}$	8.15849585	$2.51 \times 10^{-7}$	

Note. Parameters:  $s_0 = 100$ , r = 0.03, and  $\sigma = \delta s_0^\beta = 0.25$ .

**5.2.1. Modeling for VIX.** According to CBOE [12], regardless of model specifications, VIX is defined by averaging the weighted prices of out-of-the-money put and call options on S&P500 with 30-day maturity. Suppose the risk-neutral dynamics of an asset is given by

$$dS(t) = rS(t) dt + \sqrt{V(t)}S(t) dW(t),$$
(53)

where  $\{W(t)\}\$  is a standard Brownian motion; r is the risk-free rate; the process  $\{V(t)\}\$  models the stochastic variance. Based on the realized variance over the time interval  $[t, t + \Delta T]$  defined by

$$\mathrm{RV}(t, t + \Delta T) := \frac{1}{\Delta T} \int_{t}^{t + \Delta T} V(s) \, ds,$$



FIGURE 1. Uniform errors of the expansions for the CEV models.

where  $\Delta T$  corresponds to the 30-day maturity of the out-of-the-money options employed for constructing VIX, a theoretical squared VIX for modeling and pricing of derivatives on VIX (see Carr and Wu [11]) is defined by

$$\widehat{\text{VIX}}^{2}(t) = E[\text{RV}(t, t + \Delta T) \mid \mathcal{F}(t)] = \frac{1}{\Delta T} \int_{t}^{t + \Delta T} E(V(s) \mid \mathcal{F}(t)) \, ds,$$
(54)

where the expectations are taken under the risk-neutral measure and  $\{\mathcal{F}(t), t \ge 0\}$  denotes the filtration generated by the process  $\{V(t)\}$ .

The literature has witnessed various models for pricing options on VIX or related volatility derivatives. Similar to the Black-Scholes model for pricing equity and index options, Whaley [75] regarded VIX as a geometric Brownian motion with constant volatility. Grunbichler and Longstaff [32] specified the dynamics of VIX as a mean-reverting square-root process. Detemple and Osakwe [20] employed a logarithmic mean-reverting process for pricing options on volatility. Carr and Lee [9] proposed a model-free approach by using the associated variance and volatility swap rates as model inputs. Cont and Kokholm [15] studied a modeling framework for the joint dynamics of an index and a set of forward variance swap rates. In this paper, we will directly model the stochastic variance process {V(t)} in the asset dynamics (53) using the GARCH diffusion (see, e.g., Christoffersen et al. [14]) as well as its multifactor generalization to the Gatheral double lognormal stochastic volatility (DLN-SV) model (see, e.g., Gatheral [27]) and price options on VIX based on the theoretical proxy of VIX defined by (54).

**5.2.2. Valuation of options on VIX under the GARCH diffusion model.** In this subsection, we apply our expansion method to the valuation of options on VIX under the GARCH diffusion stochastic volatility model. According to Christoffersen et al. [14], the risk-neutral dynamics for the model is specified as follows. **Model 1.** *The GARCH diffusion stochastic volatility model is governed by* 

$$dV(t) = \varkappa(\theta - V(t)) dt + \sigma V(t) dW(t), \qquad V(0) = v_0 > 0,$$
(55)

where  $\varkappa$ ,  $\theta$  and  $\sigma$  are positive constants;  $\{W(t)\}$  is a standard Brownian motion.



FIGURE 2. Convergence of uniform errors.

TABLE 2	Comparisons	with	alternative	methods
IADLL 2.	Comparisons	vv i ti i	ancinative	methous.

Parameters		Alternative methods	2nd order expansion	4th order expansion	
β	K (%)	Error in implied volatility	Error in implied volatility	Error in implied volatility	
	Cor	nparison with the 3rd order app	roximation formula (2.6) in Gob	et et al. [30]	
-0.2	80	$-1.6 \times 10^{-5}$	$-1.6 \times 10^{-4}$	$-2.0 \times 10^{-6}$	
0.2	100	$-6.0 \times 10^{-6}$	$-3.2 \times 10^{-5}$	$-1.0 \times 10^{-6}$	
	120	$1.0 \times 10^{-6}$	$6.0 \times 10^{-5}$	$-8.7 \times 10^{-7}$	
	Cor	nparison with the 3rd order app	roximation formula (2.9) in Gob	et et al. [30]	
-0.8	80	$4.7 \times 10^{-4}$	$4.8 \times 10^{-4}$	$1.2 \times 10^{-4}$	
	100	$1.2 \times 10^{-4}$ $1.2 \times 10^{-4}$		$3.0 \times 10^{-5}$	
	120	$-8.4 \times 10^{-5}$	$-8.0 \times 10^{-5}$	$-8.6 \times 10^{-6}$	
	Co	mparison with the approximatio	n formula (7) in Hagan and Wo	odward [34]	
-0.5	80	$7.2 \times 10^{-5}$	$2.8 \times 10^{-4}$	$1.7 \times 10^{-5}$	
	100	$6.2 \times 10^{-5}$	$5.3 \times 10^{-5}$	$3.2 \times 10^{-6}$	
	120	$4.4 \times 10^{-5}$	$-9.5 \times 10^{-5}$	$-5.4 \times 10^{-6}$	
	С	omparison with the approximation	on formula (5.41) in Henry-Lab	ordère [35]	
-0.5	80	$7.8 \times 10^{-5}$	$2.8 \times 10^{-4}$	$1.7 \times 10^{-5}$	
	100	$6.2 \times 10^{-5}$	$5.3 \times 10^{-5}$	$3.2 \times 10^{-6}$	
	120	$4.6 \times 10^{-5}$	$-9.5 \times 10^{-5}$	$-5.4 \times 10^{-6}$	
	Cor	mparison with the approximation	n formula given in §3 of Gathers	al et al. [28]	
-0.5	80	$1.1 \times 10^{-5}$	$2.8 \times 10^{-4}$	$1.7 \times 10^{-5}$	
	100	$6.7 \times 10^{-6}$	$5.3 \times 10^{-5}$	$3.2 \times 10^{-6}$	
	120	$5.0 \times 10^{-6}$	$-9.5 \times 10^{-5}$	$-5.4 \times 10^{-6}$	

Note. Parameters:  $s_0 = 1$ , T = 10, r = 0, and  $\delta = 0.2$ .

In the SDE (55), we employ  $\varkappa$  for the speed of mean reversion,  $\theta$  for the long-term level,  $\sigma$  for the volatility of variance. Nelson [54] showed that, under the GARCH diffusion model, discrete time log returns follow a GARCH(1, 1) process of Engle and Bollerslev [24], which is popular for modeling stochastic volatility and has shown outstanding empirical performance. We note that the GARCH diffusion specification is also employed for constructing the  $\lambda$ -SABR model in Henry-Labordère [35]. According to the classification in Dai and Singleton [18], the model (55) belongs to the non-affine class, which is usually regarded to be analytically intractable and computationally challenging.

By explicitly solving  $E(V(s) | \mathcal{F}(t))$  from the fact that

$$E(V(t+\Delta T)-V(t) \mid \mathcal{F}(t)) = \varkappa \int_{t}^{t+\Delta T} (\theta - E(V(s) \mid \mathcal{F}(t))) \, ds,$$

and recalling the definition of the squared VIX in (54), we express the VIX under model (55) as a linear combination of the instantaneous variance V(t) and the long-term level  $\theta$  in the following lemma.

LEMMA 3. Under the GARCH diffusion stochastic volatility model (55), the VIX defined by (54) admits the following representation:

$$VIX(t) = \sqrt{a_1 V(t) + a_2 \theta},$$
(56)

where the coefficients are given by

$$a_1 = \frac{1}{\Delta T} \cdot \frac{1 - e^{-\varkappa \Delta T}}{\varkappa}, \quad and \quad a_2 = 1 - \frac{1}{\Delta T} \cdot \frac{1 - e^{-\varkappa \Delta T}}{\varkappa}.$$
 (57)

Thus, the price for a call option on VIX with maturity T and strike k (expressed in percentage) can be represented by risk-neutral expectation of the discounted payoff, i.e.,

$$c_0 = e^{-rT} E(\text{VIX}(T) - k)^+ = e^{-rT} E(\sqrt{a_1 V(T) + a_2 \theta} - k)^+.$$
(58)

According to the convention proposed in CBOE [12], the price per share is given by  $C_0 = 100 \times c_0$ . To apply our general expansion formulas (36) and (40), we identify V(t) as the underlying model X(t) proposed in (1). According to Lemma 3, the function for constructing VIX from X(t) is given by  $f(x) = \sqrt{a_1 x + a_2 \theta}$ . Thus, following the procedures proposed in (6), (7) and (9), we obtain the following nonlinear SDE for  $Y^{\epsilon}(t) = f(X^{\epsilon}(t))$ :

$$dY^{\epsilon}(t) = \epsilon^{2} \alpha(Y^{\epsilon}(t)) dt + \epsilon \beta(Y^{\epsilon}(t)) \circ dW(t), \qquad Y^{\epsilon}(0) = y_{0} = f(v_{0}), \tag{59}$$

where

$$\alpha(x) = \frac{\varkappa(\theta - x^2)}{2x} - \frac{\sigma^2(x^2 - a_2\theta)}{4x} \quad \text{and} \quad \beta(x) = \frac{\sigma(x^2 - a_2\theta)}{2x}.$$
 (60)

Thus, (58) can be expressed as  $c_0 = e^{-rT} E[(Y^{\epsilon}(1) - k)^+]$ . We note that the drift and volatility functions (60) both exhibit nonlinearity, which poses significant challenge on the valuation. However, such difficulty can be circumvented by our expansion.

In numerical experiments, we select a set of parameters from Barone-Adesi et al. [5]. Accordingly, the initial value for VIX is calculated as  $VIX(0) = \sqrt{a_1V(0) + a_2\theta} = 0.3$ . To provide benchmark values for comparison, we simulate the path of  $\{V(t)\}$  using Euler discretization. Thus, the initial value of an option on VIX is simulated by averaging a large number of trials, which is assumed to be the square of the number of discretization steps according to the optimal rule for allocating computational resources suggested by Duffie and Glynn [21].

As listed from the Chicago Board Options Exchange, traded options on VIX usually have relatively small maturities. The longest maturities are less than or equal to six months; and the large trading volumes are usually associated with options with small maturities, e.g., front-month options. Our numerical experiments target options with maturities ranging from one month to six months and strikes corresponding to various moneyness. In Table 3, computational results from the simulations as well as expansions of the fourth and the ninth orders are exhibited. The accuracy of the expansions can be seen from the fact that all values of the ninth order expansions lie in the 95% confidence intervals of the simulated benchmark values. In Figure 3, we plot the absolute errors of our expansions with three different orders for the four representative maturities listed in Table 3. As seen from

Parameters		Simulation		4th order expansion		9th order expansion		
Т	K	Mean	Std. err.	Asymptotic	Discrepancy	Asymptotic	Discrepancy	
1/12	25	0.048792	$5.75 \times 10^{-5}$	0.048776	$1.65  imes 10^{-5}$	0.048749	$4.33 \times 10^{-5}$	
	26	0.039403	$5.58  imes 10^{-5}$	0.039378	$2.44 \times 10^{-5}$	0.039359	$4.37 \times 10^{-5}$	
	27	0.030616	$5.27 \times 10^{-5}$	0.030623	$7.18  imes 10^{-6}$	0.030607	$9.08  imes 10^{-6}$	
	28	0.022806	$4.80 \times 10^{-5}$	0.022828	$2.26  imes 10^{-5}$	0.022813	$7.28  imes 10^{-6}$	
	29	0.016269	$4.23 \times 10^{-5}$	0.016254	$1.50  imes 10^{-5}$	0.016238	$3.13 \times 10^{-5}$	
	30	0.011018	$3.59 \times 10^{-5}$	0.011032	$1.45 \times 10^{-5}$	0.011016	$1.80  imes 10^{-6}$	
	31	0.007115	$2.93  imes 10^{-5}$	0.007135	$2.06  imes 10^{-5}$	0.007118	$2.96  imes 10^{-6}$	
	32	0.004387	$2.29 \times 10^{-5}$	0.004402	$1.56 \times 10^{-5}$	0.004384	$2.69 \times 10^{-6}$	
	33	0.002595	$1.77 \times 10^{-5}$	0.002596	$1.60  imes 10^{-6}$	0.002578	$1.67  imes 10^{-5}$	
	34	0.001469	$1.31 \times 10^{-5}$	0.001466	$2.89  imes 10^{-6}$	0.001449	$2.00 \times 10^{-5}$	
2/12	25	0.048592	$7.29 \times 10^{-5}$	0.048654	$6.14 \times 10^{-5}$	0.048490	$1.02 \times 10^{-4}$	
	26	0.039778	$6.98 \times 10^{-5}$	0.039927	$4.41 \times 10^{-5}$	0.039795	$8.53  imes 10^{-6}$	
	27	0.031879	$6.56 \times 10^{-5}$	0.031997	$1.49 \times 10^{-4}$	0.031926	$1.73 \times 10^{-5}$	
	28	0.024824	$6.03 \times 10^{-5}$	0.025011	$1.88  imes 10^{-4}$	0.024881	$5.81  imes 10^{-5}$	
	29	0.018866	$5.40 \times 10^{-5}$	0.019065	$1.99 \times 10^{-4}$	0.018933	$6.71 \times 10^{-5}$	
	30	0.014022	$4.77 \times 10^{-5}$	0.014181	$1.59 \times 10^{-4}$	0.014048	$2.57 \times 10^{-7}$	
	31	0.010184	$4.12 \times 10^{-5}$	0.010305	$1.21 \times 10^{-4}$	0.010169	$1.51 \times 10^{-5}$	
	32	0.007196	$3.49 \times 10^{-5}$	0.007330	$1.34  imes 10^{-4}$	0.007191	$4.56 \times 10^{-6}$	
	33	0.004961	$2.89 \times 10^{-5}$	0.005116	$1.55  imes 10^{-4}$	0.004973	$1.15 \times 10^{-5}$	
	34	0.003359	$2.37 \times 10^{-5}$	0.003514	$1.55  imes 10^{-4}$	0.003369	$9.89  imes 10^{-6}$	
3/12	25	0.048323	$8.14 \times 10^{-5}$	0.048865	$5.42 \times 10^{-4}$	0.048404	$8.04 \times 10^{-5}$	
	26	0.040009	$7.77 \times 10^{-5}$	0.040565	$5.56 \times 10^{-4}$	0.040127	$1.19 \times 10^{-4}$	
	27	0.032622	$7.32 \times 10^{-5}$	0.033073	$4.51 \times 10^{-4}$	0.032642	$1.94 \times 10^{-5}$	
	28	0.026041	$6.75 \times 10^{-5}$	0.026489	$4.48 \times 10^{-4}$	0.026050	$9.33 \times 10^{-6}$	
	29	0.020459	$6.15 \times 10^{-5}$	0.020853	$3.94 \times 10^{-4}$	0.020409	$4.96 \times 10^{-5}$	
	30	0.015672	$5.49 \times 10^{-5}$	0.016157	$4.85 \times 10^{-4}$	0.015709	$3.69 \times 10^{-5}$	
	31	0.011939	$4.87 \times 10^{-5}$	0.012343	$4.04  imes 10^{-4}$	0.011889	$5.08  imes 10^{-5}$	
	32	0.008974	$4.27 \times 10^{-5}$	0.009320	$3.45 \times 10^{-4}$	0.008856	$1.18  imes 10^{-4}$	
	33	0.006512	$3.64 \times 10^{-5}$	0.006974	$4.63  imes 10^{-4}$	0.006502	$1.01 \times 10^{-5}$	
	34	0.004724	$3.11 \times 10^{-5}$	0.005191	$4.67  imes 10^{-4}$	0.004710	$1.40 \times 10^{-5}$	
6/12	25	0.048042	$1.85 \times 10^{-4}$	0.051545	$3.57 \times 10^{-3}$	0.047901	$1.79 \times 10^{-4}$	
	26	0.040342	$1.77 \times 10^{-4}$	0.043774	$3.32 \times 10^{-3}$	0.040201	$2.52 \times 10^{-4}$	
	27	0.033432	$1.67 \times 10^{-4}$	0.036841	$3.35 \times 10^{-3}$	0.033290	$1.99 \times 10^{-4}$	
	28	0.027364	$1.56 \times 10^{-4}$	0.030769	$3.26 \times 10^{-3}$	0.027218	$2.97  imes 10^{-4}$	
	29	0.022140	$1.43 \times 10^{-4}$	0.025552	$3.47 \times 10^{-3}$	0.021991	$9.26 \times 10^{-5}$	
	30	0.017728	$1.31 \times 10^{-4}$	0.021149	$3.34 \times 10^{-3}$	0.017573	$2.34 \times 10^{-4}$	
	31	0.014063	$1.18  imes 10^{-4}$	0.017500	$3.38 \times 10^{-3}$	0.013903	$2.17  imes 10^{-4}$	
	32	0.011065	$1.06 \times 10^{-4}$	0.014524	$3.38 \times 10^{-3}$	0.010898	$1.61 \times 10^{-4}$	
	33	0.008640	$9.45  imes 10^{-5}$	0.012135	$3.48 \times 10^{-3}$	0.008472	$1.83  imes 10^{-4}$	
	34	0.006692	$8.37 \times 10^{-5}$	0.010241	$3.53 \times 10^{-3}$	0.006535	$1.71 \times 10^{-4}$	

TABLE 3. Numerical performance for pricing options on VIX under the GARCH diffusion model.

Note. Parameters:  $\varkappa = 2$ ,  $\theta = 0.09$ ,  $\sigma = 0.8$ ,  $v_0 = 0.09$ , and r = 0.03. Std. err.: standard error. Discrepancy: Asymptotic-Mean.

Table 3 and Figure 3, the decrease of discrepancies between the simulated benchmark value and the asymptotic expansion value resulting from the increase of orders of expansion suggests the indispensable role of high-order expansions.

**5.2.3. Valuation of options on VIX under the Gatheral double lognormal stochastic volatility model.** Similar to the previous application, we consider an extension of the GARCH diffusion model to a multifactor stochastic volatility model as follows.

Model 2. The Gatheral double log-normal stochastic volatility (DLN-SV) model is governed by

$$dV(t) = \kappa(V'(t) - V(t)) dt + \xi_1 V(t) dW_1(t), \qquad V(0) = v_0 > 0, \tag{61}$$

$$dV'(t) = \kappa'(\vartheta - V'(t)) dt + \xi_2 V'(t) [\rho \, dW_1(t) + \sqrt{1 - \rho^2} \, dW_2(t)], \qquad V'(0) = v'_0 > 0,$$

where  $-1 \le \rho \le 1$ ;  $\kappa > \kappa' > 0$ ;  $\xi_1$ ,  $\xi_2$  and  $\vartheta > 0$ ;  $\{W_1(t), W_2(t)\}$  is a standard two-dimensional Brownian motion.





FIGURE 3. Absolute errors of the expansions for the GARCH diffusion model.

Initiated by Gatheral [27], Model 2 can be regarded as a generalization of Model 1 by allowing an additional freedom in the sense that the instantaneous variance V(t) reverts to a moving intermediate level V'(t) at rate  $\kappa$ , while V'(t) reverts to the long-term level  $\vartheta$  at a slower rate  $\kappa' < \kappa$ . For various purposes, alternative multifactor stochastic volatility models have been proposed in, e.g., Duffie et al. [22], Buehler [8], Egloff et al. [23], Kaeck and Alexander [41], and Aït-Sahalia et al. [2]. Similar to the GARCH diffusion model, the DLN-SV model falls into the non-affine class.

By explicitly solving  $E(V(s) | \mathcal{F}(t))$  and  $E(V'(s) | \mathcal{F}(t))$  from the fact that

$$E(V(t + \Delta T) \mid \mathcal{F}(t)) - V(t) = \kappa \int_{t}^{t + \Delta T} (E(V'(s) \mid \mathcal{F}(t)) - E(V(s) \mid \mathcal{F}(t))) \, ds,$$
$$E(V'(t + \Delta T) \mid \mathcal{F}(t)) - V'(t) = \kappa' \vartheta \Delta T - \kappa' \int_{t}^{t + \Delta T} E(V'(s) \mid \mathcal{F}(t)) \, ds,$$

we obtain an explicit representation of VIX using a linear combination of the instantaneous variance V(t), the intermediate level V'(t), and the long-term level  $\vartheta$  in the following lemma.

LEMMA 4. Under the Gatheral DLN-SV model (61), the VIX defined by (54) admits the following representation:

$$\operatorname{VIX}(t) = \sqrt{b_1 V(t) + b_2 V'(t) + b_3 \vartheta},$$
(62)

where the coefficients are given by

$$b_1 = \frac{1}{\Delta T} \cdot \frac{1 - e^{-\kappa \Delta T}}{\kappa},\tag{63}$$

$$b_2 = \frac{1}{\Delta T} \cdot \frac{\kappa}{\kappa - \kappa'} \cdot \left( \frac{1 - e^{-\kappa'\Delta T}}{\kappa'} - \frac{1 - e^{-\kappa\Delta T}}{\kappa} \right), \tag{64}$$

$$b_3 = 1 - \frac{1}{\Delta T} \cdot \frac{1 - e^{-\kappa\Delta T}}{\kappa} - \frac{1}{\Delta T} \cdot \frac{\kappa}{\kappa - \kappa'} \cdot \left(\frac{1 - e^{-\kappa'\Delta T}}{\kappa'} - \frac{1 - e^{-\kappa\Delta T}}{\kappa}\right).$$
(65)

Parameters		Simulation		3rd order expansion		6th order expansion	
Т	K	Mean	Std. err.	Asymptotic	Discrepancy	Asymptotic	Discrepancy
1/52	8	0.043911	$3.24 \times 10^{-5}$	0.043994	$8.34 \times 10^{-5}$	0.043943	$3.28 \times 10^{-5}$
	9	0.033957	$3.23  imes 10^{-5}$	0.033999	$4.20  imes 10^{-5}$	0.033976	$1.91  imes 10^{-5}$
	10	0.024173	$3.17 \times 10^{-5}$	0.024155	$1.80  imes 10^{-5}$	0.024171	$1.45  imes 10^{-6}$
	11	0.015298	$2.90  imes 10^{-5}$	0.015246	$5.21  imes 10^{-5}$	0.015274	$2.44 \times 10^{-5}$
	12	0.008402	$2.37 \times 10^{-5}$	0.008381	$2.08 \times 10^{-5}$	0.008407	$5.51  imes 10^{-6}$
	13	0.004056	$1.73 \times 10^{-5}$	0.040170	$3.89  imes 10^{-5}$	0.004044	$1.19  imes 10^{-5}$
	14	0.001726	$1.14  imes 10^{-5}$	0.001700	$2.54  imes 10^{-5}$	0.001729	$3.47  imes 10^{-6}$
	15	0.000667	$7.10  imes 10^{-6}$	0.000650	$1.73 \times 10^{-5}$	0.006732	$6.04  imes 10^{-6}$
	16	0.000242	$4.20  imes 10^{-6}$	0.000240	$2.02 \times 10^{-6}$	0.000247	$5.19 imes10^{-6}$
	17	0.000083	$2.36  imes 10^{-6}$	0.000092	$8.90  imes 10^{-6}$	0.000086	$3.09  imes 10^{-6}$
2/52	8	0.045213	$4.41 \times 10^{-5}$	0.045338	$1.25 \times 10^{-4}$	0.045218	$5.18 \times 10^{-6}$
	9	0.035326	$4.38 \times 10^{-5}$	0.035440	$4.43 \times 10^{-5}$	0.035318	$8.57  imes 10^{-6}$
	10	0.025829	$4.24 \times 10^{-5}$	0.025927	$8.81 \times 10^{-5}$	0.025875	$4.57 \times 10^{-5}$
	11	0.017635	$3.87 \times 10^{-5}$	0.017653	$1.63 \times 10^{-4}$	0.017610	$2.56 \times 10^{-5}$
	12	0.011162	$3.31 \times 10^{-5}$	0.011219	$1.18  imes 10^{-4}$	0.011178	$1.53 \times 10^{-5}$
	13	0.006681	$2.69 \times 10^{-5}$	0.006722	$1.35 \times 10^{-4}$	0.006680	$2.59 \times 10^{-7}$
	14	0.003813	$2.07 \times 10^{-5}$	0.003845	$1.53  imes 10^{-4}$	0.003800	$1.27 \times 10^{-5}$
	15	0.002090	$1.54 \times 10^{-5}$	0.002117	$1.52  imes 10^{-4}$	0.002085	$4.27 \times 10^{-6}$
	16	0.001089	$1.13  imes 10^{-5}$	0.000990	$9.90  imes 10^{-5}$	0.001077	$1.15  imes 10^{-5}$
	17	0.000542	$8.20  imes 10^{-6}$	0.000524	$1.79  imes 10^{-5}$	0.000549	$7.60  imes 10^{-6}$
3/52	8	0.046746	$5.33 \times 10^{-5}$	0.046658	$8.82 \times 10^{-5}$	0.046662	$8.40 \times 10^{-5}$
	9	0.036806	$5.27 \times 10^{-5}$	0.036550	$2.55 \times 10^{-4}$	0.036781	$2.43 \times 10^{-5}$
	10	0.027602	$5.07 \times 10^{-5}$	0.027241	$3.61 \times 10^{-4}$	0.027624	$2.13 \times 10^{-5}$
	11	0.019723	$4.68 \times 10^{-5}$	0.019309	$4.14 \times 10^{-4}$	0.019688	$3.53 \times 10^{-5}$
	12	0.013479	$4.13 \times 10^{-5}$	0.013066	$4.13  imes 10^{-4}$	0.013452	$4.34 \times 10^{-5}$
	13	0.008896	$3.52 \times 10^{-5}$	0.008481	$4.19  imes 10^{-4}$	0.008853	$4.72 \times 10^{-5}$
	14	0.005684	$2.89  imes 10^{-5}$	0.005290	$3.94  imes 10^{-4}$	0.005673	$1.18  imes 10^{-5}$
	15	0.003598	$2.33 \times 10^{-5}$	0.003159	$4.39  imes 10^{-4}$	0.003553	$4.57  imes 10^{-5}$
	16	0.002246	$1.90  imes 10^{-5}$	0.001805	$4.41 \times 10^{-4}$	0.002230	$1.56  imes 10^{-5}$
	17	0.001294	$1.50 \times 10^{-5}$	0.001016	$2.78  imes 10^{-4}$	0.001274	$2.00 \times 10^{-5}$
1/12	8	0.047775	$7.93 \times 10^{-5}$	0.047590	$1.58 \times 10^{-4}$	0.047730	$1.67 \times 10^{-5}$
	9	0.038101	$7.86  imes 10^{-5}$	0.037438	$6.63 \times 10^{-4}$	0.038063	$3.82 \times 10^{-5}$
	10	0.028960	$7.63 \times 10^{-5}$	0.028238	$7.23 \times 10^{-4}$	0.028915	$4.55 \times 10^{-5}$
	11	0.021208	$7.25  imes 10^{-5}$	0.020447	$7.61  imes 10^{-4}$	0.021121	$8.68  imes 10^{-5}$
	12	0.014986	$6.67  imes 10^{-5}$	0.014264	$7.22  imes 10^{-4}$	0.014924	$6.21  imes 10^{-5}$
	13	0.010356	$6.07  imes 10^{-5}$	0.009616	$7.39  imes 10^{-4}$	0.010279	$7.69  imes 10^{-5}$
	14	0.007028	$5.96  imes 10^{-5}$	0.006258	$7.70  imes 10^{-4}$	0.006945	$8.27  imes 10^{-5}$
	15	0.004652	$5.90  imes 10^{-5}$	0.003900	$7.53  imes 10^{-4}$	0.004609	$4.32 \times 10^{-5}$
	16	0.003153	$5.85  imes 10^{-5}$	0.002298	$8.55  imes 10^{-4}$	0.003048	$1.04  imes 10^{-4}$
	17	0.002144	$5.72 \times 10^{-5}$	0.001282	$8.62  imes 10^{-4}$	0.002034	$1.09  imes 10^{-4}$

TABLE 4. Numerical performance for pricing options on VIX under the DLN-SV model.

*Note.* Parameters:  $\kappa = 5.5$ ,  $\xi_1 = 2.6$ ,  $v_0 = 0.0137$ ,  $\kappa' = 0.1$ ,  $\vartheta = 0.078$ ,  $\xi_2 = 0.44$ ,  $v'_0 = 0.0208$ ,  $\rho = 0.57$ , and r = 0.04. Std. err.: standard error. Discrepancy: Asymptotic-Mean.

Thus, the price of a call option on VIX with maturity T and strike k can be represented as

$$c_0 = e^{-rT} E \left( \sqrt{b_1 V(t) + b_2 V'(t) + b_3 \vartheta} - k \right)^+.$$
(66)

To apply the general formulas (40) and (36) for expansion, we identify (V(t), V'(t)) as a two-dimensional general model  $X(t) = (X_1(t), X_2(t))$  as proposed in (1). The function for constructing the VIX (62) from X(t) is given by  $f(x_1, x_2) = \sqrt{b_1 x_1 + b_2 x_2 + b_3 \vartheta}$ . Thus, following the procedures proposed in (6), (7) and (9), we obtain the following nonlinear SDE for  $Y^{\epsilon}(t) = (Y_1^{\epsilon}(t), Y_2^{\epsilon}(t))$  with  $Y_1^{\epsilon}(t) = f(X_1^{\epsilon}(t), X_2^{\epsilon}(t))$  and  $Y_2^{\epsilon}(t) = X_2^{\epsilon}(t)$ :

$$dY^{\epsilon}(t) = \epsilon^{2} \alpha(Y^{\epsilon}(t)) dt + \epsilon \beta(Y^{\epsilon}(t)) \circ dW(t), \qquad Y^{\epsilon}(0) = y_{0} = f(v_{0}),$$

where

$$\alpha(x) \equiv \alpha((x_1, x_2)) = \left(\frac{1}{2x_1} \left[ (b_1 \kappa - b_2 \kappa' - \frac{1}{2} b_2 \xi_2^2) x_2 - (\kappa + \frac{1}{2} \xi_1^2) (x_1^2 - b_2 x_2 - b_3 \vartheta) + b_2 \kappa' \vartheta \right] \\ \kappa'(\vartheta - x_2) - \frac{1}{2} \xi_2^2 x_2 \right],$$

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FIGURE 4. Absolute errors of the expansions for the Gatheral DLN-SV model.

and

$$\beta(x) \equiv \beta((x_1, x_2)) = \begin{pmatrix} \frac{1}{2x_1} [\xi_1(x_1^2 - b_2 x_2 - b_3 \vartheta) + \rho \xi_2 b_2 x_2] & \frac{1}{2x_1} \sqrt{1 - \rho^2} \xi_2 b_2 x_2 \\ \rho \xi_2 x_2 & \sqrt{1 - \rho^2} \xi_2 x_2 \end{pmatrix}$$

Thus, (58) can be expressed as  $c_0 = e^{-rT} E[(Y_1^{\epsilon}(1) - k)^+].$ 

Owing to the highly volatile feature of VIX, the front-month (maturity less then or equal to one month) options on VIX have been widely used as important and effective hedging tools. For instance, by rolling one-month VIX options, VXTH (VIX tail hedge strategy) proposed in CBOE [13] has shown satisfactory performance for managing portfolio downside risk. Accordingly, we illustrate the applicability of our expansion in the valuation of options on VIX with relatively small maturities. In the numerical experiments, we employ the set of parameters given in Gatheral [27]. Accordingly, the initial value for VIX is calculated as VIX (0) =  $\sqrt{b_1 V(0) + b_2 V'(0) + b_3 \vartheta} = 0.1226$ . To provide benchmark values for comparison, we simulate the path of  $\{(V(t), V'(t))\}$  using Euler discretization. In Table 4, computational results for the simulated values as well as the third and the sixth orders of our expansions are exhibited. The accuracy of the expansion can be seen from the fact that all the sixth order expansion values lie in the 95% confidence intervals of the four representative maturities listed in Table 4. As seen from Table 4 and Figure 4, the decrease of discrepancies between the simulated benchmark value and the asymptotic expansion value resulting from the increase of expansion orders suggests the applicability of our method. In particular, for valuation of options on VIX with longer maturities, we could seek for desirable accuracy by implementing higher-order expansions.

**6.** Concluding remarks. Enlightened by the theory of Watanabe [74] for analyzing generalized random variables and its further development in Yoshida [76], Takahashi [61, 62] as well as Kunitomo and Takahashi [48, 49] etc., we focus on a wide range of multivariate diffusion models and propose a general probabilistic method of small-time asymptotic expansions for approximating option price in simple closed-form up to an

arbitrary order. To explicitly construct correction terms, we introduce an efficient algorithm and novel closedform formulas for calculating conditional expectation of multiplication of iterated stochastic integrals, which are potentially useful in a wider range of topics in applied probability and stochastic modeling for operations research. The performance of our method is illustrated through various models nested in the CEV type processes. With an application in pricing options on VIX under the GARCH diffusion and its multifactor generalization to the Gatheral double lognormal stochastic volatility models, we demonstrate the versatility of our method in dealing with analytically intractable non-Lévy and non-affine models. The robustness of the method is theoretically supported by justifying uniform convergence of the expansion over the whole set of parameters.

In summary, our method may become a convenient and efficient tool for option valuation under a wide range of diffusion models with flexible specification. In particular, because of the fast development of computing technology in terms of speed and storage capacity, symbolic implementation of high-order expansions will become increasingly more feasible and will thus render desirable accuracy for various purposes.

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#### Appendix A. Proofs for Section 3

#### A.1. Proof of Proposition 1.

PROOF. Indeed, we have

$$\Omega_{k}(z) = \sum_{(n,\mathbf{r}(n))\in\mathcal{R}_{k}} \frac{1}{n!} E\left(\frac{\partial^{(n)}T}{\partial x^{n}}(Z_{0})Z_{r_{1}}Z_{r_{2}}\dots Z_{r_{n}}\right)$$
  
=  $E(1\{Z_{0} \ge z\}Z_{k}) + \sum_{n \ge 2, (n,\mathbf{r}(n))\in\mathcal{R}_{k}} \frac{1}{n!} E(\delta^{(n-2)}(Z_{0}-z)Z_{r_{1}}Z_{r_{2}}\dots Z_{r_{n}}).$  (A1)

We deduce that

$$E(1\{Z_0 \ge z\}Z_k) = \int_{-\infty}^{\infty} E(1\{Z_0 \ge z\}Z_k \mid Z_0 = x)\phi(x) \, dx = \int_{z}^{\infty} E(Z_k \mid Z_0 = x)\phi(x) \, dx,$$

where the integrand can be further explicitly calculated as

$$E(Z_k \mid Z_0 = x) = D(y_0)E(Y_{k+1,1} \mid Z_0 = x)$$
  
=  $D(y_0)E\left(\sum_{\|\mathbf{i}\| = k+1} C_{\mathbf{i},1}(y_0)J_{\mathbf{i}}(1) \mid Z_0 = x\right) = D(y_0)\sum_{\|\mathbf{i}\| = k+1} C_{\mathbf{i},1}(y_0)E(J_{\mathbf{i}}(1) \mid B(1) = x).$ 

Thus, we obtain that

$$E(1\{Z_0 \ge z\}Z_k) = D(y_0) \sum_{\|\mathbf{i}\| = k+1} C_{\mathbf{i},1}(y_0) \int_{z}^{\infty} E(J_{\mathbf{i}}(1) \mid B(1) = x) \phi(x) dx = D(y_0) \sum_{\|\mathbf{i}\| = k+1} C_{\mathbf{i},1}(y_0) \mathcal{F}(P_{(\mathbf{i})})(z).$$
(A2)

On the other hand, by the integration-by-parts formula involving the Dirac delta function (see, e.g., section 2.6 in Kanwal [42]) we deduce that,

$$\begin{split} E(\delta^{(n-2)}(Z_0-z)Z_{r_1}Z_{r_2}\dots Z_{r_n}) &= \int_{-\infty}^{\infty} \delta^{(n-2)}(x-z)E(Z_{r_1}Z_{r_2}\dots Z_{r_n} \mid Z_0 = x)\phi(x) \, dx \\ &= (-1)^{n-2} \int_{-\infty}^{\infty} \delta(x-z) \frac{\partial^{(n-2)}}{\partial x^{n-2}} \Big[ E(Z_{r_1}Z_{r_2}\dots Z_{r_n} \mid Z_0 = x)\phi(x) \Big] \, dx \\ &= (-1)^{n-2} \frac{\partial^{(n-2)}}{\partial z^{n-2}} \Big[ E(Z_{r_1}Z_{r_2}\dots Z_{r_n} \mid Z_0 = z)\phi(z) \Big], \end{split}$$

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where the conditional expectation is calculated as

$$E(Z_{r_1}Z_{r_2}\dots Z_{r_n} | Z_0 = z) = D(y_0)^n E(Y_{r_1+1,1}Y_{r_2+1,1}\dots Y_{r_n+1,1} | Z_0 = z)$$
  
=  $D(y_0)^n E\left(\prod_{j=1}^n \sum_{\|\mathbf{i}_w\|=r_j+1} C_{\mathbf{i},1}(y_0)J_{\mathbf{i}}(1) | Z_0 = z\right)$   
=  $D(y_0)^n \sum_{\substack{\|\mathbf{i}_w\|=r_w+1, \\ w=1,2,\dots,n}} \left(\prod_{w=1}^n C_{\mathbf{i}_w,1}(y_0)\right) E\left(\left(\prod_{w=1}^n J_{\mathbf{i}_w}(1)\right) | B(1) = z\right).$ 

Using the differential operator (31), we obtain that

$$\frac{\partial^{(n-2)}}{\partial z^{n-2}} \left[ E(Z_{r_1} Z_{r_2} \dots Z_{r_n} \mid Z_0 = z) \phi(z) \right] = D(y_0)^n \sum_{\substack{\|\mathbf{i}_w\| = r_w + 1, \\ w = 1, 2, \dots, n}} \left( \prod_{w=1}^n C_{\mathbf{i}_w, 1}(y_0) \right) \mathcal{D}^{n-2}(P_{(\mathbf{i}_1, \mathbf{i}_2, \dots, \mathbf{i}_n)})(z) \phi(z).$$
(A3)

Thus, the formula (36) follows from plugging (A2) and (A3) into (A1).  $\Box$ 

A.2. Proof of Proposition 2. Without loss of generality and in order to simplify the notations, we consider the case of  $f(x) \equiv x$ , in which the transform in (9) becomes an identity and the dynamics (7) and (10) coincide with each other, i.e.,

> $X^{\epsilon}(t) \equiv Y^{\epsilon}(t),$  $x_0 \equiv y_0$ ,  $\mu(x) \equiv \alpha(x),$ and  $\sigma(x) \equiv \beta(x).$

For general specifications of f(x) satisfying Assumption 3, the proof follows from a straightforward adaption of the following arguments. For simplicity, we avoid such notational complication.

Based on Assumption 2, we introduce the following uniform upper bounds. For  $k \ge 1$ , let  $\mu_k$  and  $\sigma_k$  be the uniform upper bounds of the kth order derivative of  $\mu$  and  $\sigma$ , respectively, i.e.,

$$|\partial^{(k)}\mu(x;\theta)/\partial x^k| \le \mu_k \quad \text{and} \quad |\partial^{(k)}\sigma(x;\theta)/\partial x^k| \le \sigma_k, \tag{A4}$$

for  $(x, \theta) \in \mathbb{R}^m \times \Theta$ . Also, for any arbitrary  $x_0$ , let  $\mu_0$  and  $\sigma_0$  denote the uniform upper bounds of  $|\mu(x_0; \theta)|$ and  $|\sigma(x_0; \theta)|$  on  $\theta \in \Theta$ , respectively, i.e.,

$$|\mu(x_0; \theta)| \le \mu_0$$
 and  $|\sigma(x_0; \theta)| \le \sigma_0$ , (A5)

for any  $\theta \in \Theta$ . To establish the uniform convergence rate in Proposition 2, we introduce the following lemma. When the dependence of parameters is emphasized, we express  $Y^{\epsilon}(1)$  as  $Y^{\epsilon}(1; \theta, y_0)$  and express the standardized random variable  $Z^{\epsilon}$  defined in (21) as  $Z^{\epsilon}(\theta, y_0) = D(y_0)(Y^{\epsilon}(1; \theta, y_0) - y_0)/\sqrt{T}$  in this appendix. Let  $S(\subset E)$  be an arbitrary compact subset of the state space of the diffusion X.

LEMMA 5. Under Assumption 2, the following asymptotic expansion holds uniformly in  $(\theta, y_0) \in \Theta \times S$ :

$$\left\| Z^{\epsilon}(\theta, y_0) - \sum_{k=0}^{J} \frac{1}{k!} \frac{\partial^{(k)} Z^{\epsilon}(\theta, y_0)}{\partial \epsilon^k} \right|_{\epsilon=0} \epsilon^k \left\|_{D^p_s} = \mathcal{O}(\epsilon^{J+1}),$$

for any  $J \in N$ ,  $p \ge 1$  and  $s \in N$ , where  $\|\cdot\|_{D_s^p}$  is the  $D_s^p$ -Malliavin norm (see, e.g., section 1.5 in Nualart [55])

PROOF OF LEMMA 5. The proof of this lemma follows the similar lines of argument for proving Theorem 7.1 in Malliavin and Thalmaier [51]. Thus, it is omitted.  $\Box$ 

PROOF OF PROPOSITION 2. First, we note that the diffusion matrix (12) satisfies

$$\beta(y_0) = \beta((f(x_{01}, x_{02}, \dots, x_{0m}), x_{02}, \dots, x_{0m})) \equiv M\sigma(x_0),$$

where M is a matrix defined by

$$M = \begin{pmatrix} \frac{\partial f(x_0)}{\partial x_1} & \frac{\partial f(x_0)}{\partial x_2} & \cdots & \frac{\partial f(x_0)}{\partial x_m} \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}_{m \times m}.$$

Since we assume  $\partial f / \partial x_1 \neq 0$ , it follows that Assumption 1 is equivalent to the positive definite property of the matrix  $\beta(y_0)\beta(y_0)^T$ , i.e.,

$$\det A(x_0) = \det(\sigma(x_0)\sigma(x_0)^T) > 0 \quad \Longleftrightarrow \quad \det(\beta(y_0)\beta(y_0)^T) > 0.$$
(A6)

According to the theory of Watanabe [74] and Yoshida [76, 77, 78], the uniform nondegeneracy of the standardized random variable (21) and the convergence of the expansion (23) clarified in Lemma 5 yields the validity of the expansion (28) in the following sense:

$$\sup_{\boldsymbol{\epsilon} \in \boldsymbol{R}, \, \boldsymbol{x}_0 \in \boldsymbol{S}, \, \boldsymbol{\theta} \in \boldsymbol{\Theta}} \left| E[(\boldsymbol{Z}^{\boldsymbol{\epsilon}} - \boldsymbol{z})^+] - \sum_{k=0}^J \Omega_k(\boldsymbol{z}) \boldsymbol{\epsilon}^k \right| \le c' \boldsymbol{\epsilon}^{J+1},$$

for any  $J \in N$  and some positive constant c'. Based on (24), we have

$$\sup_{z \in R, \, x_0 \in S, \, \theta \in \Theta} \left| \sqrt{T} e^{-rT} D(y_0)^{-1} E[(Z^{\epsilon} - z)^+] - \sqrt{T} e^{-rT} D(y_0)^{-1} \sum_{k=0}^J \Omega_k(z) \epsilon^k \right| \le c \epsilon^{J+1},$$

for some constant c. Therefore, by plugging in (25) and  $\epsilon = \sqrt{T}$ , we obtain that

$$\sup_{K \in \mathbb{R}^+, \, x_0 \in S, \, \theta \in \Theta} \left| V(0) - \sqrt{T} e^{-rT} D(y_0)^{-1} \sum_{k=0}^J \Omega_k(D(y_0)(K - y_{01})/\sqrt{T}) T^{k/2} \right| \le c T^{(J+1)/2}. \quad \Box$$

**Appendix B. Proofs for §4** This appendix is devoted to proving Proposition 3. We begin by introducing some preparatory notions (e.g., pair partition) in combinatorial analysis in Appendix B.1, which is followed by a useful lemma in Appendix B.2. Then, based on pair partitions, a formula for calculating (50) is proposed in Appendix B.3. Finally, a proof for Proposition 3 is given in Appendix B.4 based on all the previous development.

**B.1. Paring partitions.** First, we introduce the following notions involving partitions of an index set *X*. A *partition* is a collection of pair-wise disjoint and nonempty subsets whose union is *X*. In particular, suppose that *X* contains an even number of elements; a partition is called a *pair partition*, if each of its sets has exactly two elements. For example,  $\{\{1, 2\}, \{3, 4\}, \{5, 6\}\}$  is a pair partition of the set  $\{1, 2, 3, 4, 5, 6\}$ . For an arbitrary set *Y*, let  $\mathbb{A}(X, Y)$  denote the collection of pair partitions of the set *X* satisfying that none of its elements is *Y*. In particular, for *Y* being an empty set  $\phi$ , we simply abbreviate  $\mathbb{A}(X, Y)$  as  $\mathbb{A}(X)$ . For example,

$$\mathbb{A}(\{1, 2, 3, 4\}, \{2, 3\}) = \{\{\{1, 2\}, \{3, 4\}\}, \{\{1, 3\}, \{2, 4\}\}\},\$$

and

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$$\mathbb{A}(\{1, 2, 3, 4\}) = \{\{\{1, 2\}, \{3, 4\}\}, \{\{1, 3\}, \{2, 4\}\}, \{\{1, 4\}, \{2, 3\}\}\}$$

For more details about set partitions, readers are referred to, e.g., Brualdi [7]. For an arbitrary pair-partition  $\mathcal{P} = \{\{l_1, l_2\}, \{l_3, l_4\} \cdots \{l_{2n-1}, l_{2n}\}\}$  for some integer set, we correspondingly define

$$\mathcal{P}(i) := \left\{ \{i_{l_1}, i_{l_2}\}, \{i_{l_3}, i_{l_4}\} \cdots \{i_{l_{2n-1}}, i_{l_{2n}}\} \right\}$$

for  $i_{l_1}, i_{l_2}, i_{l_3}, \dots, i_{l_{2n-1}}, i_{l_{2n}} \in \{0, 1, 2, \dots, d\}$ . Also, we define a *characterization* of  $\mathcal{P}(i)$  as

$$\chi(\mathscr{P}(i)) := \delta_{i_{l_1}i_{l_2}} \delta_{i_{l_3}i_{l_4}} \dots \delta_{i_{l_{2n-1}}i_{l_{2n}}},\tag{B1}$$

where  $\delta_{ij}$  is the Kronecker delta function taking value 1 if i = j, and 0 otherwise. In particular, for the empty set  $\emptyset$ , we let  $\chi(\emptyset) = 1$ .

**B.2. A useful lemma.** We propose a useful lemma by generalizing Proposition 5.2.3 in Kloeden and Platen [46].

LEMMA 6. Let  $\mathbf{i} = (i_1, i_2, \ldots, i_l) \in \{0, 1, 2, \ldots, d\}^l$  be an index satisfying that  $i_r > 0$  if and only if  $r \in \{j_1, j_2, \ldots, j_n\} \subset \{1, 2, \ldots, l\}$  for some integer n. For any arbitrary integer  $k = 1, 2, \ldots, and i_{l+1}, i_{l+2}, \ldots, i_{l+k} \in \{1, 2, \ldots, d\}$ , we have

$$E\left(\prod_{1\leq s\leq k} W_{i_{l+s}}(1)I_{(i_1,i_2,\ldots,i_l)}(1)\right) = \sum_{\mathscr{S}\in\mathbb{A}(\{j_1,j_2,\ldots,j_n,l+1,l+2,\ldots,l+k\},\{j_1,j_2,\ldots,j_n\})} \frac{\chi(\mathscr{S}(i))}{l!},$$
(B2)

if  $k \ge n$  and k + n is even;

$$E\left(\prod_{1\leq s\leq k} W_{i_{l+s}}(1)I_{(i_1,i_2,\ldots,i_l)}(1)\right) = 0,$$

otherwise.

Before giving a proof to this lemma, we provide three concrete examples in what follows.

EXAMPLE 1. For  $(i_1, i_2, \dots, i_6) \in \{1, 2, \dots, m\}^6$ , we have

$$E[W_{i_1}(1)W_{i_2}(1)W_{i_3}(1)I_{(i_4,i_5)}(1)] = 0, \quad \text{and} \quad E[W_{i_1}(1)W_{i_2}(1)I_{(i_4,i_5,i_6)}(1)] = 0,$$

and

$$\begin{split} E[W_{i_1}(1)W_{i_2}(1)W_{i_3}(1)I_{(i_4,i_5,i_6)}(1)] \\ &= \frac{1}{6} \Big( \delta_{i_1i_4} \delta_{i_2i_5} \delta_{i_3i_6} + \delta_{i_1i_4} \delta_{i_2i_6} \delta_{i_3i_5} + \delta_{i_1i_5} \delta_{i_2i_4} \delta_{i_3i_6} + \delta_{i_1i_5} \delta_{i_2i_6} \delta_{i_3i_4} + \delta_{i_1i_6} \delta_{i_2i_5} \delta_{i_3i_4} + \delta_{i_1i_6} \delta_{i_2i_4} \delta_{i_3i_5} \Big), \end{split}$$

as well as

$$\begin{split} E[W_{i_1}(1)W_{i_2}(1)W_{i_3}(1)I_{(i_4,i_5,0,i_6)}(1)] \\ &= \frac{1}{24} \Big( \delta_{i_1i_4} \delta_{i_2i_5} \delta_{i_3i_6} + \delta_{i_1i_4} \delta_{i_2i_6} \delta_{i_3i_5} + \delta_{i_1i_5} \delta_{i_2i_4} \delta_{i_3i_6} + \delta_{i_1i_5} \delta_{i_2i_6} \delta_{i_3i_4} + \delta_{i_1i_6} \delta_{i_2i_5} \delta_{i_3i_4} + \delta_{i_1i_6} \delta_{i_2i_4} \delta_{i_3i_5} \Big). \end{split}$$

PROOF OF LEMMA 6. The main idea of the proof is based on iterative applications of Proposition 5.2.3 in Kloeden and Platen [46], which asserts that a multiplication of a Brownian multiplier to an iterated Itô stochastic integral can be expressed as a linear combination of iterated Itô stochastic integrals. For ease of exposition, we introduce a linear operator as follows. For any  $i \in \{1, 2, ..., d\}$ , we define

$$\mathcal{W}_i := \mathcal{W}_i^P + \mathcal{W}_i^R,$$

where  $\mathcal{W}_{i}^{P}$  is a plug operator defined by

$$\mathscr{W}_{i}^{P}(I_{(i_{1},i_{2},\ldots,i_{l})}(t)) := \sum_{1 \le \nu \le l+1} I_{(i_{1},\ldots,i_{\nu-1},i,i_{\nu},\ldots,i_{l})}(t);$$
(B3)

 $\mathcal{W}_{i}^{R}$  is a replacement operator defined by

$$\mathscr{W}_{i}^{R}(I_{(i_{1},i_{2},\ldots,i_{l})}(t)) := \sum_{1 \le \nu \le l} \delta_{ii_{\nu}} I_{(i_{1},\ldots,i_{\nu-1},0,i_{\nu+1},\ldots,i_{l})}(t),$$
(B4)

for an arbitrary iterated Itô integral  $I_{(i_1,i_2,\ldots,i_l)}(t)$ . Thus, Proposition 5.2.3 in Kloeden and Platen [46] can be recasted as

$$W_{i}(t)I_{(i_{1},i_{2},\ldots,i_{l})}(t) \equiv \mathcal{W}_{i}(I_{(i_{1},i_{2},\ldots,i_{l})}(t)) \equiv \mathcal{W}_{i}^{P}(I_{(i_{1},i_{2},\ldots,i_{l})}(t)) + \mathcal{W}_{i}^{R}(I_{(i_{1},i_{2},\ldots,i_{l})}(t)).$$
(B5)

Iterative applications of (B5) yield

$$\prod_{1 \le s \le k} W_{i_{l+s}}(1) I_{(i_1, i_2, \dots, i_l)}(1) = \mathcal{W}_{i_{l+1}}(\mathcal{W}_{i_{l+2}}(\dots (\mathcal{W}_{i_{l+k}}(I_{(i_1, i_2, \dots, i_l)}(1)), \dots)),$$
(B6)

which can be eventually written as a linear combination of iterated (stochastic) integrals.

When k < n, we claim that

$$E\left(\prod_{1\le s\le k} W_{i_{l+s}}(1)I_{(i_1,i_2,\ldots,i_l)}(1)\right) = 0.$$
(B7)

Indeed, in this case, there are fewer Brownian multipliers for performing replacement than the nonzero elements in  $(i_1, i_2, \ldots, i_l)$ . Thus, every term in a linear combination form of (B6) will contain stochastic integrations with respect to Brownian motions. Therefore, (B7) follows from the martingale property of stochastic integrals.

When  $k \ge n$ , we begin by observing the following basic fact. The total number of nonzero indices in the iterated (stochastic) integrals on the right-hand side of (B3) is n + 1; the total number of nonzero indices in the iterated (stochastic) integrals on the right-hand side of (B4) is n - 1. Iterative application of this fact to (B6) leads to the following observation. Assuming k + n (the total number of nonzero indices in  $W_{i_{l+1}}(1)W_{i_{l+2}}(1)\ldots W_{i_{l+k}}(1)I_{(i_1,i_2,\ldots,i_l)}(1)$ ) is an odd number, the operation (B6) renders a linear combination of iterated (stochastic) integrals, each of which has an odd number of nonzero indices. Therefore, we obtain (B7). Alternatively, we consider the case where k + n is an even number. We note that, in (B5), the consumptions of nonzero indices in  $(i_1, i_2, \ldots, i_l)$  must be based on replacement operations as defined in (B4). The way to create iterated Lebesgue integrals in the operations (B3) and (B4) can be characterized as follows: each nonzero

index in  $\{j_1, j_2, \ldots, j_n\}$  must be replaced by zero via multiplication with a Brownian multiplier; in the rest k - noperations, (k - n)/2 must be chosen as a plug; the others are thereby performed as replacement.

Each iterated Lebesgue integration in the linear combination form of (B6) must be associated to a pair partition in  $\mathbb{A}(\{j_1, j_2, \dots, j_n, l+1, l+2, \dots, l+k\}, \{j_1, j_2, \dots, j_n\})$ . Indeed, without loss of generality, we consider an arbitrary pair partition, e.g.,

Such a choice corresponds to the following operations:

- Perform the plug operations using the Brownian multipliers  $W_{i_{l+n+2}}, W_{i_{l+n+4}}, \ldots, W_{i_{l+k}}$ .
- Perform the replacement operations using the Brownian multipliers  $W_{i_{l+n+1}}^{i_{l+n+2}}(1), W_{i_{l+n+3}}(1), \dots, W_{i_{l+k-1}}(1)$ . Replace  $i_{j_1}, i_{j_2}, \dots, i_{j_n}$  by zeros via the replacement operations using the Brownian multipliers  $W_{i_{l+1}}(1), W_{i_{l+2}}(1), \dots, W_{i_{l+n}}(1).$

Therefore, we have that

$$E\left(\prod_{1\leq s\leq k}W_{i_{l+s}}(1)I_{(i_1,i_2,\ldots,i_l)}(1)\right) = \sum_{\mathscr{G}\in\mathbb{A}(\{j_1,j_2,\ldots,j_n,l+1,l+2,\ldots,l+k\},\{j_1,j_2,\ldots,j_n\})}c(\mathscr{G})\chi(\mathscr{G}(i)),$$
(B9)

where  $c(\mathcal{S})$  is a coefficient (to be determined) associated with a pair-partition  $\mathcal{S}$ . In particular, owing to the commutativity, we observe that

$$\prod_{1 \le s \le k} W_{i_{l+s}}(1) I_{(i_1, i_2, \dots, i_l)}(1) \equiv W_{i_{l+1}}(1) W_{i_{l+2}}(1) \cdots W_{i_{l+n}}(1) (W_{i_{l+n+1}}(1) W_{i_{l+n+3}}(1) \cdots W_{i_{l+k-1}}(1)) \times (W_{i_{l+n+2}}(1) W_{i_{l+n+4}}(1) \cdots W_{i_{l+k}}(1)) I_{(i_1, i_2, \dots, i_l)}(1).$$

Thus, the term in (B9) generated by the operations corresponding to the pair-partition (B8) is given by

$$c(\mathscr{Q})\chi(\mathscr{Q}(i)) = E\Big[\mathscr{W}_{i_{l+1}}^{(R)}(\mathscr{W}_{i_{l+2}}^{(R)}(\cdots \mathscr{W}_{i_{l+n}}^{(R)}(\mathscr{W}_{i_{l+n+1}}^{(R)}(\cdots \mathscr{W}_{i_{l+n+3}}^{(R)}(\cdots \mathscr{W}_{i_{l+k-1}}^{(R)}(\mathscr{W}_{i_{l+n+2}}^{(P)}(\mathscr{W}_{i_{l+n+4}}^{(P)}(\cdots \mathscr{W}_{i_{l+n+4}}^{(P)}(I_{(i_{1},i_{2},\ldots,i_{l})}(1))\cdots))))))\Big].$$
(B10)

We note that the iterated Lebesgue integrals resulting from expanding (B10) all have length l + (k - n)/2. We also observe that

$$\mathcal{W}_{i_{l+n+2}}^{(P)}\left(\mathcal{W}_{i_{l+n+4}}^{(P)}(\cdots \mathcal{W}_{i_{l+k}}^{(P)}(I_{(i_{1},i_{2},\ldots,i_{l})}(1))\cdots)\right) = \sum_{\mathbf{i}\in\mathscr{B}(\{i_{1},\ldots,i_{l},i_{l+n+2},i_{l+n+4},\ldots,i_{l+k}\},\{i_{1},i_{2},\ldots,i_{l}\})}I_{\mathbf{i}}(1),$$

where  $\mathcal{B}(x, y)$  collects all permutations of an ordered index set x without shuffling the order of indices in its subset y (for example,  $\mathscr{B}(\{i_1, i_2, i_3, i_4\}, \{i_1, i_2, i_3\}) = \{\{i_1, i_2, i_3, i_4\}, \{i_1, i_2, i_4, i_3\}, \{i_1, i_4, i_2, i_3\}, \{i_4, i_1, i_2, i_3\}\})$ . Therefore, we have

$$c(@) = \left| \mathscr{B}\left(\{i_1, \dots, i_l, i_{l+n+2}, i_{l+n+4}, \dots, i_{l+k}\}, \{i_1, i_2, \dots, i_l\}\right) \right| \\ \times \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{l+(k-n)/2-1}} dt_{l+(k-n)/2} \cdots dt_2 dt_1 \\ = \binom{l+(k-n)/2}{(k-n)/2} \times \binom{k-n}{2}! \times \frac{1}{(l+(k-n)/2)!} = \frac{1}{l!}.$$

Hence, (B2) is proved.  $\Box$ 

**B.3.** A formula based on pairing partition. Based on Lemma 6, we establish the following expression for a conditional expectation of an arbitrary iterated Itô integral using pair partition.

LEMMA 7. For any arbitrary index  $\mathbf{i} = (i_1, i_2, \dots, i_n)$  with  $i_1, i_2, \dots, i_n \in \{0, 1, \dots, d\}$ , we have

$$E[I_{\mathbf{i}}(1) | W(1) = \mathbf{x}] = \frac{1}{n!} \sum_{j=0}^{\lfloor n/2 \rfloor} (-1)^{j} \sum_{L_{n-2j} = \{l_{1}, l_{2}, \dots, l_{n-2j}\} \subset N_{n}} \sum_{\mathscr{S} \in \mathbb{A}(N_{n} \setminus L_{n-2j})} \chi(\mathscr{S}(i)) x_{i_{l_{1}}} x_{i_{l_{2}}}, \dots, x_{i_{l_{n-2j}}},$$
(B11)

where  $N_n$  denotes the integer set  $\{1, 2, ..., n\}$ ;  $L_k = \{l_1, l_2, ..., l_k\}$  denotes any arbitrary subset of  $N_n$  with k elements;  $\lfloor x \rfloor$  denotes the largest integer less than or equal to x;  $x_i$  is assumed to be 1 for i = 0.

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PROOF OF LEMMA 7. This proof starts from an explicit construction of the conditional distribution of  $(W(t) | W(1) = \mathbf{x})$  using Brownian bridges. By the construction of Brownian bridge (see Karatzas and Shreve [43, p. 358]), we obtain the following distributional identity, for any k = 1, 2, ..., d,

$$(W_k(t) \mid W(1) = \mathbf{x}) \stackrel{\mathcal{D}}{=} (W_k(t) \mid W_k(1) = x_k) \stackrel{\mathcal{D}}{=} BB_k^x(t) := \mathcal{B}_k(t) - t\mathcal{B}_k(1) + tx_k,$$

where  $\mathcal{B}_k$ 's are independent Brownian motions. In other words,  $\{BB_k^x(t), 0 \le t \le 1\}$  is distributed as a Brownian bridge starting from 0 at time 0 and ending at  $x_k$  at time 1. For ease of exposition, we also introduce  $\mathcal{B}_0(t) \equiv 0$  and  $x_0 = 1$ . Therefore, we have

$$E[I_{\mathbf{i}}(1)|W(1) = \mathbf{x}] = E\left(\int_{0}^{1}\int_{0}^{t_{1}}\cdots\int_{0}^{t_{n-1}}d(\mathscr{B}_{i_{n}}(t_{n}) - t_{n}\mathscr{B}_{i_{n}}(1) + t_{n}x_{i_{n}})\cdots d(\mathscr{B}_{i_{1}}(t_{1}) - t_{1}\mathscr{B}_{i_{1}}(1) + t_{1}x_{i_{1}})\right).$$
(B12)

By expanding the right-hand side of (B12) and collecting terms according to monomials of  $x_i$ 's, we obtain that

$$E[I_{\mathbf{i}}(1) | W(1) = \mathbf{x}] = \sum_{k=0}^{n} \sum_{\{l_1, l_2, \dots, l_k\} \subset N_n = \{1, 2, \dots, n\}} c(l_1, l_2, \dots, l_k) x_{i_{l_1}} x_{i_{l_2}}, \dots, x_{i_{l_k}},$$

where the coefficients are determined by

$$c(l_{1}, l_{2}, \dots, l_{k}) := E \int_{0}^{1} \int_{0}^{t_{1}} \cdots \int_{0}^{t_{n-1}} d(\mathscr{B}_{i_{n}}(t_{n}) - t_{n}\mathscr{B}_{i_{n}}(1)) \cdots d(\mathscr{B}_{i_{l_{k}+1}}(t_{l_{k}+1}) - t_{l_{k}+1}\mathscr{B}_{i_{l_{k}+1}}(1)) dt_{l_{k}}$$
  

$$\cdot d(\mathscr{B}_{i_{l_{k}-1}}(t_{l_{k}-1}) - t_{l_{k}-1}\mathscr{B}_{i_{l_{k}-1}}(1)) \cdots d(\mathscr{B}_{i_{l_{2}+1}}(t_{l_{2}+1}) - t_{l_{2}+1}\mathscr{B}_{i_{l_{2}+1}}(1)) dt_{l_{2}}$$
  

$$\cdot d(\mathscr{B}_{i_{l_{2}-1}}(t_{l_{2}-1}) - t_{l_{2}-1}\mathscr{B}_{i_{l_{2}-1}}(1)) \cdots d(\mathscr{B}_{i_{l_{1}+1}}(t_{l_{1}+1}) - t_{l_{1}+1}\mathscr{B}_{i_{l_{1}+1}}(1)) dt_{l_{1}}$$
  

$$\cdot d(\mathscr{B}_{i_{l_{1}-1}}(t_{l_{1}-1}) - t_{l_{1}-1}\mathscr{B}_{i_{l_{1}-1}}(1)) \cdots d(\mathscr{B}_{i_{1}}(t_{1}) - t_{1}\mathscr{B}_{i_{1}}(1)).$$
(B13)

To explicitly calculate (B13), we define the following index mapping. For an index  $\mathbf{i} = (i_1, i_2, \dots, i_n)$ , an integer set  $L_k = \{l_1, l_2, \dots, l_k\}$ , and any subset  $M \subset N_n \setminus L_k$ , let

$$\varphi(\mathbf{i};L_k,M)=(j_1,j_2,\ldots,j_n),$$

where, for any r = 1, 2, ..., n,

$$j_r = 0$$
, if  $r \in L_k \cup M$ ;  $j_r = i_r$ , otherwise

Thus, we have

$$c(l_1, l_2, \dots, l_k) = E\left(\sum_{M \subset N_n \setminus L_k} (-1)^{|M|} I_{\varphi(\mathbf{i}; L_k, M)}(1) \prod_{r \in M} \mathscr{B}_{l_r}(1)\right)$$
$$= \sum_{M \subset N_n \setminus L_k} (-1)^{|M|} E\left(I_{\varphi(\mathbf{i}; L_k, M)}(1) \prod_{r \in M} \mathscr{B}_{l_r}(1)\right)$$

By Lemma 6, we have

$$E\left(I_{\varphi(\mathbf{i};\,L_k,\,M)}(1)\prod_{r\in M}\mathscr{B}_{i_r}(1)\right)=\frac{1}{n!}\sum_{\mathscr{S}\in\mathbb{A}(N_n\setminus L_k,\,N_n\setminus(L_k\cup M))}\chi(\mathscr{S}(i)),$$

if n - k is an even number and  $|M| \ge (n - k)/2$ , where |S| denotes the cardinality of a set S;

$$E\left(I_{\varphi(\mathbf{i}; L_k, M)}(1) \prod_{r \in M} \mathscr{B}_{i_r}(1)\right) = 0,$$

otherwise.

So, if n - k is an odd number, we have  $c(l_1, l_2, ..., l_k) = 0$ . If n - k is an even number, we deduce that

$$\begin{split} c(l_1, l_2, \dots, l_k) &= \frac{1}{n!} \sum_{M \subset N_n \setminus L_k} (-1)^{|M|} \sum_{\mathscr{P} \in \mathbb{A}(N_n \setminus L_k, N_n \setminus (L_k \cup M))} \chi(\mathscr{P}(i)) \\ &= \frac{1}{n!} \sum_{r=(n-k)/2}^{n-k} (-1)^r \sum_{\mathscr{P} \in \mathbb{A}(N_n \setminus L_k)} \sum_{M \in \{M: |M| = r, \mathscr{P} \in \mathbb{A}(N_n \setminus L_k, N_n \setminus (L_k \cup M))\}} \chi(\mathscr{P}(i)) \\ &= \frac{1}{n!} \sum_{\mathscr{P} \in \mathbb{A}(N_n \setminus L_k)} \sum_{r=(n-k)/2}^{n-k} (-1)^r \binom{(n-k)/2}{r-(n-k)/2} 2^{n-k-r} \chi(\mathscr{P}(i)) \\ &= \frac{1}{n!} \sum_{\mathscr{P} \in \mathbb{A}(N_n \setminus L_k)} (-1)^{(n-k)/2} \chi(\mathscr{P}(i)), \end{split}$$

where we have employed combinatorics to calculate the cardinality of a set, i.e.,

$$\left|\left\{M: |M|=r, \mathcal{P} \in \mathbb{A}(N_n \setminus L_k, N_n \setminus (L_k \cup M))\right\}\right| = \binom{(n-k)/2}{r-(n-k)/2} 2^{n-k-r}.$$

Hence, the formula (B11) follows immediately.  $\Box$ 

**B.4. Proof of Proposition 3.** Finally, we give a proof to Proposition 3 based on Lemma 7.

PROOF OF PROPOSITION 3. We express (B11) in an alternative way according to monomials of  $x_1, \ldots, x_d$ . Thus, combinatorial analysis and the definition (B1) indicate that the term  $x_1^{k_1} \ldots x_d^{k_d}$  for some  $k_1, k_2, \ldots, k_d \in \{1, 2, \ldots, n\}$  appears in (B11) if and only if  $n_i(1) - k_1, n_i(2) - k_2, \ldots, n_i(d) - k_d$  are all even integers. In this case, the total number of appearances of the term  $x_1^{k_1} \ldots x_d^{k_d}$  is given by

$$\prod_{l=1}^{d} \left[ |\mathbb{A}(N_{n_{\mathbf{i}}(l)-k_{l}})| \binom{n_{\mathbf{i}}(l)}{k_{l}} \right],$$

where  $|\mathbb{A}(N_n)|$  is the total number of all possible pair partitions of the set  $N_n = \{1, 2, ..., n\}$ . It is straightforward to observe that

$$|\mathbb{A}(N_n)| \equiv \nu(n) = \prod_{k=0}^{(n/2)-1} \binom{n-2k}{2} / \binom{n}{2}!,$$

for an arbitrary even integer *n*. Also, any arbitrary pair partition in  $\mathbb{A}(N_{n_i(l)-k_l})$  has exactly  $(n_i(l) - k_l)/2$  elements. Therefore, we obtain the formula (51).  $\Box$ 

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