One-parameter extension of the Doi-Peliti formalism and its relation with orthogonal polynomials

Jun Ohkubo*

Graduate School of Informatics, Kyoto University, Yoshida Hon-machi, Sakyo-ku, Kyoto-shi, Kyoto 606-8501, Japan

(Received 17 August 2012; published 23 October 2012)

An extension of the Doi-Peliti formalism for stochastic chemical kinetics is proposed. Using the extension, path-integral expressions consistent with previous studies are obtained. In addition, the extended formalism is naturally connected to orthogonal polynomials. We show that two different orthogonal polynomials, i.e., Charlier polynomials and Hermite polynomials, can be used to express the Doi-Peliti formalism explicitly.

DOI: 10.1103/PhysRevE.86.042102 PACS number(s): 05.40.−a, 82.20.−w, 02.50.Ey

Introduction. Stochastic chemical kinetics has been widely used in various research areas. For example, reaction-diffusion systems based on the stochastic chemical kinetics have been used in nonequilibrium physics [1]. In addition, recent development of experimental techniques enables us to observe various reactions in a cell in detail, and it has been clarified that some chemical reactions in cells should be treated as systems with discrete states; continuous approximation cannot be used [2].

The Doi-Peliti formalism [3–5] is known as a useful method to treat classical stochastic processes, such as the stochastic chemical kinetics and reaction-diffusion processes. The Doi-Peliti formalism has a similar structure with second quantization methods in quantum mechanics, and many methods and concepts developed in quantum mechanics are available in order to study the classical stochastic processes; we can use perturbation calculations [6], renormalization group analysis [1], and system-size expansion [7]. However, there are some unclear points of the formalism: are there concrete representations for the state vectors and operators used in the Doi-Peliti formalism? While it has been pointed out that the Doi-Peliti formalism is equivalent to generating function approach or Poisson representation [8], the correspondence would not be unique. If we have various concrete representations for the Doi-Peliti formalism, it is possible to choose an adequate one depending on one's objectives. For example, efficient statistical inference for stochastic reaction processes are necessary to analyze experimental data adequately, and it is important to employ some approximations (for example, see [9]), and numerical evaluations play an important role. It will be expected that an adequate choice of expressions in the Doi-Peliti formalism gives a tractable and efficient computational method for the parameter estimations.

In this Brief Report, we first propose an extension of the Doi-Peliti formalism. While the extension includes an additional parameter, the introduction of the parameter does not change the coherent-state path-integral formula; all analytical techniques in previous works are available. The extension affects only the concrete expressions for state vectors in the formalism. Second, we point out that the one-parameter extension of the Doi-Peliti formalism is naturally connected to orthogonal polynomials. We find that at least two different orthogonal polynomials, the Hermite polynomials and the Charlier polynomials, are available to describe the state vectors in the formalism. The Hermite polynomials consist of continuous variables, and, in contrast, the Charlier polynomials are composed of discrete variables. While there would be other polynomials to describe the Doi-Peliti formalism, these two famous polynomials will become a basis for future applications of the Doi-Peliti formalism.

Doi-Peliti formalsm. In the Doi-Peliti formalism, the following bosonic creation operator $a^\dagger$ and annihilation operators a are used:

$$[a,a^\dagger] \equiv aa^\dagger - a^\dagger a = 1, \quad [a,a] = [a^\dagger,a^\dagger] = 0, \qquad (1)$$

where $[\cdot,\cdot]$ is the commutator, and the actions of the creation and annihilation operators for ket vectors $|n\rangle$ are defined as

$$a^\dagger|n\rangle = |n+1\rangle, \quad a|n\rangle = n|n-1\rangle. \qquad (2)$$

Here, the vacuum state $|0\rangle$ is characterized by $a|0\rangle = 0$. While the actions of two operators on the ket vectors are defined as Eq. (2), actions on bra vectors $\langle n|$ are defined as follows:

$$\langle n|a = \langle n+1|, \quad \langle n|a^\dagger = \langle n-1|n. \qquad (3)$$

The inner product for the bra and ket vectors is given as

$$\langle m|n\rangle = n!\,\delta_{m,n}, \qquad (4)$$

where $\delta_{m,n}$ is the Kronecker δ.

When we consider a master equation for a chemical kinetics with only one variable, a probability $P(n,t)$, with which we find n particles at time t, is developed according to the master equation [10]. The remarkable idea of the Doi-Peliti formalism is the usage of a single vector $|\psi(t)\rangle$ which is a collection of a series of an infinite number of $P(n,t)$:

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} P(n,t)|n\rangle. \qquad (5)$$

Using the vector $|\psi(t)\rangle$, the master equation for $P(n,t)$ is rewritten in a compact form:

$$\frac{\partial}{\partial t}|\psi(t)\rangle = L(a^\dagger,a)|\psi(t)\rangle, \qquad (6)$$

where $L(a^\dagger,a)$ is a time-evolution operator for $|\psi(t)\rangle$. Because of the similarity with quantum mechanics, the Doi-Peliti formalism is also called the second-quantization method or the field-theoretic approach.

Here, we briefly explain some basic definitions for a coherent-state path-integral expression, which are especially useful in the Doi-Peliti formalism. In order to derive the

*ohkubo@i.kyoto-u.ac.jp

path-integral expression, coherent states and a decomposition of unity play essential roles. The coherent states are defined as

$$|z\rangle \equiv e^{za^\dagger}|0\rangle = \sum_{n=0}^{\infty} \frac{z^n}{n!}|n\rangle, \tag{7}$$

$$\langle z| \equiv \langle 0|e^{z^* a} = \sum_{n=0}^{\infty} \frac{(z^*)^n}{n!}\langle n|, \tag{8}$$

where z is a complex number, and z^* is the complex conjugate of z. Using the coherent states, the decomposition of unity is obtained as follows:

$$\begin{aligned}\mathbf{1} &= \sum_{n=0}^{\infty} \frac{1}{n!}|n\rangle\langle n| = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{1}{m!}|n\rangle\langle m|\delta_{n,m} \\ &= \int \frac{d^2 z}{\pi}\, e^{-|z|^2}|z\rangle\langle z|\,,\end{aligned} \tag{9}$$

where we used

$$\delta_{n,m} = \int \frac{d^2 z}{\pi n!}\, e^{-|z|^2} z^{*m} z^n\,, \tag{10}$$

with the integration measure $d^2 z = d(\mathrm{Re}\, z) d(\mathrm{Im}\, z)$. Using the decomposition of unity, it is straightforward to obtain the path-integral expression; for details, see Ref. [1].

Note that there are some differences between the Doi-Peliti formalism and quantum mechanics. One of them is the calculation scheme for expectation values of observables; an expectation value of observables in the Doi-Peliti formalism is obtained by using a projection state:

$$\langle \mathcal{P}| \equiv \langle 0|\mathrm{e}^{a} = \sum_{n=0}^{\infty} \frac{1}{n!}\langle n|. \tag{11}$$

For example, the average of n is given by $\sum_{n=0}^{\infty} n P(n,t) = \langle \mathcal{P}|a^\dagger a|\psi(t)\rangle$.

Extension of Doi-Peliti formalism. Starting from the same commutation relation (1) and the same definitions for the ket vectors (2), it is possible to add one parameter λ to the formalism. That is, we define the following inner product instead of Eq. (4):

$$\langle m|n\rangle = \lambda^n n!\,\delta_{m,n}. \tag{12}$$

According to the replacement of Eq. (4) with Eq. (12), the actions of the creation and annihilation operators on bra vectors $\langle n|$ change as follows:

$$\langle n|a = \langle n+1|\lambda^{-1}, \quad \langle n|a^\dagger = \langle n-1|n\lambda. \tag{13}$$

The derivation of Eq. (13) is as follows: First, we have $\langle n+1|a^\dagger|n\rangle = \langle n+1|n+1\rangle = (n+1)\lambda^{n+1}$ because $a^\dagger|n\rangle = |n+1\rangle$. Second, we assume the action of the creation operator on the bra vector as $\langle n+1|a^\dagger = \langle n|\alpha$, where α is a scalar value. Then, $\langle n+1|a^\dagger|n\rangle = \alpha\langle n|n\rangle = \alpha n!\lambda^n$, and we have $\alpha = (n+1)\lambda$. Hence, the second equality in Eq. (13) is obtained. Using the similar discussions, the first equality in Eq. (13) is easily checked.

We here note that the path-integral expression must not be changed due to the above one-parameter extension because the final expression of the path-integrals consists of integrals only for parameters in the coherent states, i.e., z and z^*; the final expression does not depend on the definition of $|n\rangle$ and $\langle n|$. (For the similar reason, a definition of the "inclusive" scalar product is not changed, which is introduced in Ref. [11] and more useful compared with Eq. (12) in the applications and discussions for factorial moments.) Actually, there is no need to change the definitions of the projection state and the coherent states. Since the actions of the creation and annihilation operators for the bra vectors are modified as Eq. (13), we have $|n\rangle = (a^\dagger)^n|0\rangle$ and $\langle n| = \langle 0|(a\lambda)^n$. Hence, from the same definitions with the usual Doi-Peliti formalism, we obtain slightly different expressions for the projection state and the coherent states when we write them explicitly using the bra vectors $\langle n|$ as follows:

$$\langle \mathcal{P}| \equiv \langle 0|e^{a} = \sum_{n=0}^{\infty} \frac{1}{\lambda^n}\frac{1}{n!}\langle n|, \tag{14}$$

$$|z\rangle \equiv e^{za^\dagger}|0\rangle = \sum_{n=0}^{\infty} \frac{1}{n!} z^n|n\rangle, \tag{15}$$

$$\langle z| \equiv \langle 0|e^{z^* a} = \sum_{n=0}^{\infty} \frac{1}{n!}\langle n|\left(\frac{z^*}{\lambda^n}\right)^n. \tag{16}$$

The above expressions suggest that there is no need to change the definitions of the projection states and coherent states. In addition, the decomposition of unity is calculated as

$$\mathbf{1} = \sum_{n=0}^{\infty} \frac{1}{\lambda^n}\frac{1}{n!}|n\rangle\langle n| = \int \frac{d^2 z}{\pi}\, e^{-|z|^2}|z\rangle\langle z|. \tag{17}$$

The unity in the extended Doi-Peliti formalism has the same expression with the usual Doi-Peliti formalism in terms of the coherent states, and therefore we obtain the same path-integral expressions even in the one-parameter extension, as expected.

In the following discussions, we restrict the additional parameter λ as a positive real variable, i.e., $\lambda > 0$, in order to see the connection to the generating function approach and the orthogonal polynomials.

Expression from generating function. If we set $\lambda = 1$ in the extended Doi-Peliti formalism, an explicit representation based on the generating function approach has been already known [8]. That is, we interpret the creation and annihilation operators as

$$a^\dagger \equiv x, \quad a \equiv \frac{d}{dx}, \tag{18}$$

and the ket and bra vectors are written as follows:

$$|n\rangle \equiv x^n, \quad \langle m| \equiv \int dx\, \delta(x)\left(\frac{d}{dx}\right)^m (\cdot), \tag{19}$$

where $\delta(x)$ is the Dirac's δ function.

As far as we know, no one has found other explicit representations for the Doi-Peliti formalism. Although the correspondence in Eqs. (18) and (19) has been used to discuss duality relations in stochastic processes [12], it uses the Dirac's δ function, and hence it may be intractable for numerical computations. In what follows, we give two representations based on orthogonal polynomials.

Hermite polynomials. One of the representations is obtained from the Hermite polynomials [13]. The Hermite polynomials are defined as

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}, \tag{20}$$

where $n \in \mathbb{N}, x \in \mathbb{R}$. Introducing a scaling variable $\lambda \in \mathbb{R}$, we define the following rescaled Hermite polynomials:

$$\tilde{H}_n^{(\lambda)}(x) \equiv \sqrt{\left(\frac{\lambda}{2}\right)^n} H_n\left(\frac{x}{\sqrt{2\lambda}}\right). \tag{21}$$

Using the property of the Hermite polynomials, it is straightforward to verify the following three-term recurrence formula:

$$\tilde{H}_{n+1}^{(\lambda)}(x) = x\tilde{H}_n^{(\lambda)}(x) - \lambda n \tilde{H}_{n-1}^{(\lambda)}(x). \tag{22}$$

In addition, the rescaled Hermite polynomials satisfy the following orthogonality relation:

$$\int_{-\infty}^{+\infty} \tilde{H}_n^{(\lambda)}(x)\tilde{H}_m^{(\lambda)}(x)\mu^{(\lambda)}(x)dx = \lambda^n n!\delta_{n,m}, \tag{23}$$

where

$$\mu^{(\lambda)}(x) = \frac{1}{\sqrt{2\pi\lambda}} e^{-x^2/(2\lambda)}. \tag{24}$$

As one can easily see, the orthogonality relation (23) corresponds to the inner product (12) in the one-parameter extension of the Doi-Peliti formalism. Actually, if we define

$$|n\rangle \equiv \tilde{H}_n^{(\lambda)}(x), \quad \langle n| \equiv \int_{-\infty}^{\infty} dx \mu^{(\lambda)}(x)\tilde{H}_n^{(\lambda)}(x), \tag{25}$$

$$a^\dagger \equiv x - \lambda\frac{d}{dx}, \quad a \equiv \frac{d}{dx}, \tag{26}$$

all properties in the one-parameter extension of the Doi-Peliti formalism are recovered. For example, the action of the creation operators on the bra vector, $\langle n|a^\dagger = \langle n-1|n\lambda$, is verified by using the recurrence formula (22) and a partial integral.

Charlier polynomials. Another representation is obtained from the Charlier polynomials [13]. The definition of the monic Charlier polynomials is

$$C_n^{(\lambda)}(x) = \sum_{k=0}^{n} (-\lambda)^{n-k} x^{(k)} \binom{n}{k}, \tag{27}$$

where $x^{(k)} = x(x-1)\cdots(x-k+1)$ and $n \in \mathbb{N}, x \in \mathbb{N}$. Note that the variable x is not a real value but a natural number, which is different from the Hermite polynomials. The Charlier polynomials satisfy the recurrence formula

$$C_{n+1}^{(\lambda)}(x) = (x-n-\lambda)C_n^{(\lambda)}(x) - \lambda n C_{n-1}^{(\lambda)}(x) \tag{28}$$

and the orthogonality relation

$$\sum_{x=0}^{\infty} C_n^{(\lambda)}(x) C_m^{(\lambda)}(x) \frac{\lambda^x}{x!} e^{-\lambda} = \lambda^n n! \delta_{m,n}. \tag{29}$$

We here introduce the following definitions for the bra and ket vectors:

$$|n\rangle \equiv C_n^{(\lambda)}(x), \quad \langle n| \equiv \sum_{x=0}^{\infty} \frac{\lambda^x}{x!} e^{-\lambda} C_n^{(\lambda)}(x). \tag{30}$$

In order to recover the properties of the one-parameter extension of the Doi-Peliti formalism, we define the creation and annihilation operators as

$$a^\dagger f(x) \equiv x f(x-1) - \lambda f(x), \quad a f(x) \equiv f(x+1) - f(x). \tag{31}$$

Some techniques in discrete mathematics are needed to verify Eqs. (2) and (13) for the above definitions. It is well known that the difference operator [14]

$$\Delta u(x) \equiv u(x+1) - u(x) \tag{32}$$

acts on the Charlier polynomials as

$$\Delta C_n^{(\lambda)}(x) = C_n^{(\lambda)}(x+1) - C_n^{(\lambda)}(x) = n C_{n-1}^{(\lambda)}(x), \tag{33}$$

so that $a|n\rangle = n|n-1\rangle$ is verified. In addition, the combination of the recurrence formula (28) and the difference equation [13],

$$-nC_n^{(\lambda)}(x) = \lambda C_n^{(\lambda)}(x+1) - (x+a)C_n^{(\lambda)}(x) + xC_n^{(\lambda)}(x-1), \tag{34}$$

gives

$$C_{n+1}^{(\lambda)}(x) = xC_n^{(\lambda)}(x-1) - \lambda C_n^{(\lambda)}(x), \tag{35}$$

which corresponds to $a^\dagger|n\rangle = |n+1\rangle$. In order to check $\langle n|a^\dagger = \langle n-1|n\lambda$, a partial summation is available. Using the shift operator defined as

$$\mathrm{E}u(x) \equiv u(x+1), \tag{36}$$

the partial summation is given by [14]

$$\sum u\Delta v = uv - \sum \Delta u \mathrm{E} v. \tag{37}$$

We here note that $a^\dagger|n\rangle$ is interpreted as

$$xC_n^{(\lambda)}(x-1) - \lambda C_n^{(\lambda)}(x) = -x\Delta C_n^{(\lambda)}(x-1) + xC_n^{(\lambda)}(x) - \lambda C_n^{(\lambda)}(x).$$

Hence, $\langle n|a^\dagger|m\rangle$ is expressed as

$$\begin{aligned}
&\sum_{x=0}^{\infty} \frac{e^{-\lambda}\lambda^x}{x!} C_n^{(\lambda)}(x)\left[-x\Delta C_m^{(\lambda)}(x-1) + xC_m^{(\lambda)}(x) - \lambda C_m^{(\lambda)}(x)\right] \\
&= \left[\frac{e^{-\lambda}\lambda^x}{x!} C_n^{(\lambda)}(x)(-x)C_m^{(\lambda)}(x-1)\right]_{x=0}^{x=\infty} \\
&\quad + \sum_{x=0}^{\infty}\left[\Delta\left\{\frac{e^{-\lambda}\lambda^x}{x!} C_n^{(\lambda)}(x)x\right\} \mathrm{E}C_m^{(\lambda)}(x-1)\right. \\
&\quad \left. + \frac{e^{-\lambda}\lambda^x}{x!} C_n^{(\lambda)}(x)\left\{xC_m^{(\lambda)}(x) - \lambda C_m^{(\lambda)}(x)\right\}\right] \\
&= \sum_{x=0}^{\infty}\left[\left\{\frac{e^{-\lambda}\lambda^{x+1}}{x!} C_n^{(\lambda)}(x+1) - \frac{e^{-\lambda}\lambda^x}{(x-1)!} C_n^{(\lambda)}(x)\right\} C_m^{(\lambda)}(x)\right. \\
&\quad \left. + \frac{e^{-\lambda}\lambda^x}{x!} C_n^{(\lambda)}(x)\left\{xC_m^{(\lambda)}(x) - \lambda C_m^{(\lambda)}(x)\right\}\right] \\
&= \sum_{x=0}^{\infty} \frac{e^{-\lambda}\lambda^x}{x!} \lambda\left\{C_n^{(\lambda)}(x+1) - C_n^{(\lambda)}(x)\right\} C_m^{(\lambda)}(x) \\
&= \sum_{x=0}^{\infty} \frac{e^{-\lambda}\lambda^x}{x!} \lambda n C_{n-1}^{(\lambda)}(x) C_m^{(\lambda)}(x),
\end{aligned} \tag{38}$$

where we used Eq. (33) to obtain the final equality. Hence, the action of the creation operator $a^\dagger$ on the bra vector, $\langle n|a^\dagger = \langle n-1|n\lambda$, is verified. The action of the annihilation operator a on the bra vector, $\langle n|a = \langle n+1|\lambda^{-1}$, can be checked in a similar manner.

Concluding remarks. We have presented a one-parameter extension of the Doi-Peliti formalism, and the extended formalism is deeply related to orthogonal polynomials. Although the correspondence with the generating function approach has already been known, essentially different representations for the one-parameter extension of the Doi-Peliti formalism have been obtained; especially, the Charlier polynomials consist of only discrete variables, and hence this representation may be useful in order to construct efficient numerical methods. The additional parameter λ would be used to choose an adequate basis, which is important in numerical evaluations. In addition, it has been shown that the Charlier polynomials have an explicit relation with a certain type of birth-death process, and an adequate choice of the additional parameter is necessary to express the transition probability in a simple form [15]. It would be an important future work to reveal relationships between these mathematical results and the Doi-Peliti formalism.

In this Brief Report, we discussed only univariate cases, and researches for multivariate cases will be interesting future works. Although a naive treatment would be the usage of a simple product of univariate polynomials, there may be suitable multivariate polynomials for some specific cases.

The Doi-Peliti formalism has wide applications, as shown in previous many studies. We believe that the extension and representations in this Brief Report can also be used for applications of the Doi-Peliti formalism.

Acknowledgment. This work was supported in part by a grant-in-aid for scientific research (Grant No. 20115009) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan.

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