An application of geometric methods to the one-step processes stochastization

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The International Conference “Mathematical Modeling and Computational Physics, 2017,”
July 3–7, 2017

One-Step Processes

- The representation of the state vectors (combinatorial approach).
- The representation of the occupation numbers (operator approach).

1. The abstract indices notation is used in this work. Under this notation a tensor as a whole object is denoted just as an index (e.g., x^i), components are denoted by underlined index (e.g., $x^{\underline{i}}$).
2. We will adhere to the following agreements. Latin indices from the middle of the alphabet (i, j, k) will be applied to the space of the system state vectors. Latin indices from the beginning of the alphabet (a) will be related to the Wiener process space. Greek indices (α) will set a number of different interactions in kinetic equations.

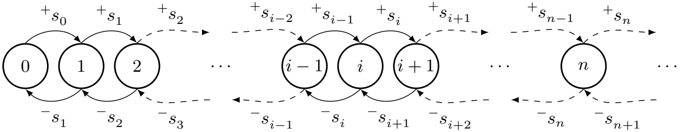

Figure 1. One-step process

Two Possibilities

- Computational approach — the solution of the master equation with help of perturbation theory.
- Modeling approach — the approximate models are obtained in the form of Fokker–Planck and Langevin equations.

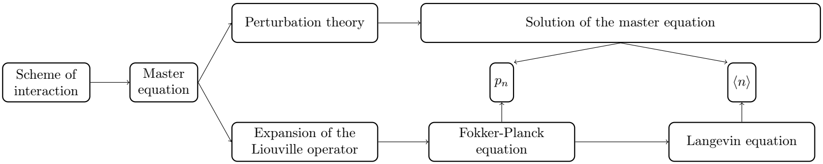

Figure 2. The general structure of the methodology

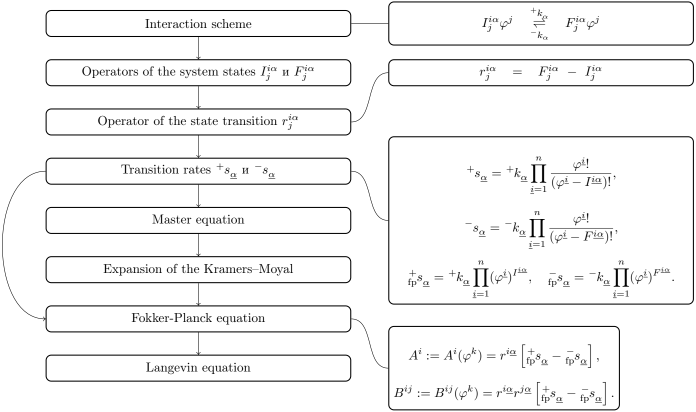

Figure 3. Combinatorial modeling approach

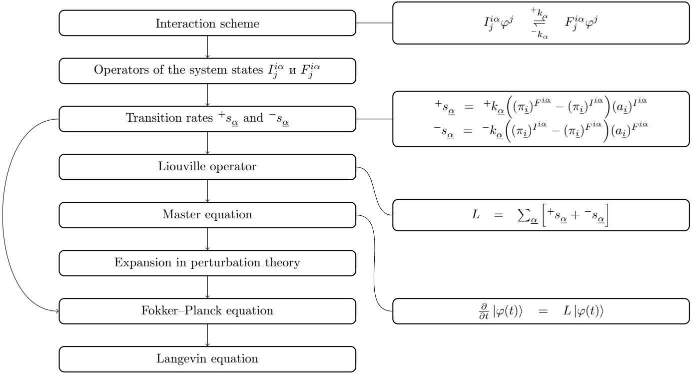

Figure 4. Operator modeling approach

$$I^{i\underline{\alpha}}_{j}\varphi^{j} \underset{{}^{-}k_{\underline{\alpha}}}{\overset{{}^{+}k_{\underline{\alpha}}}{\rightleftharpoons}} F^{i\underline{\alpha}}_{j}\varphi^{j}, \qquad \underline{\alpha} = \overline{1, s},$$

the Greek indices specify the number of interactions and Latin are the system order. The coefficients ${}^{+}k_{\underline{\alpha}}$ and ${}^{-}k_{\underline{\alpha}}$ have meaning intensity (speed) of interaction.

The state transition is given by the operator:

$$r^{i\underline{\alpha}}_{j} = F^{i\underline{\alpha}}_{j} - I^{i\underline{\alpha}}_{j}.$$

One step interaction $\underline{\alpha}$ in forward and reverse directions can be written as

$$\begin{aligned} \varphi^{i} &\to \varphi^{i} + r^{i\underline{\alpha}}_{j} \varphi^{j}, \\ \varphi^{i} &\to \varphi^{i} - r^{i\underline{\alpha}}_{j} \varphi^{j}. \end{aligned}$$

We can also write not in the form of vector equations but in the form of sums:

$$I^{i\underline{\alpha}}_{j}\varphi^{j}\delta_{i} \underset{{}^{-}k_{\underline{\alpha}}}{\overset{{}^{+}k_{\underline{\alpha}}}{\rightleftharpoons}} F^{i\underline{\alpha}}_{j}\varphi^{j}\delta_{i},$$

where $\delta_{\underline{i}} = (1, \dots, 1)$.
Also the following notation will be used:

$$I^{i\underline{\alpha}} := I^{i\underline{\alpha}}_{j}\delta^{j}, \quad F^{i\underline{\alpha}} := F^{i\underline{\alpha}}_{j}\delta^{j}, \quad r^{i\underline{\alpha}} := r^{i\underline{\alpha}}_{j}\delta^{j}.$$

Master equation

$$\frac{\partial p(\varphi_2, t_2 | \varphi_1, t_1)}{\partial t} = \int \Big[w(\varphi_2 | \psi, t_2) p(\psi, t_2 | \varphi_1, t_1) - \\ - w(\psi | \varphi_2, t_2) p(\varphi_2, t_2 | \varphi_1, t_1) \Big] \,\mathrm{d}\psi \,,$$

where $w(\varphi|\psi, t)$ is the probability of transition from the state ψ to the state φ for unit time.

Master equation for subensemble

$$\frac{\partial p(\varphi, t)}{\partial t} = \int \left[w(\varphi|\psi, t) p(\psi, t) - w(\psi|\varphi, t) p(\varphi, t) \right] \mathrm{d}\psi \, .$$

Discrete master equation

$$\frac{\partial p_n(t)}{\partial t} = \sum_m [w_{nm} p_m(t) - w_{mn} p_n(t)],$$

where the p_n is the probability of the system to be in a state n at time t, w_{nm} is the probability of transition from the state m into the state n per unit time.

Transition probabilities

$$w_{\underline{\alpha}}(\varphi^i|\psi^i, t) = {}^{+}s_{\underline{\alpha}}\delta_{\varphi^i,\psi^i+1} + {}^{-}s_{\underline{\alpha}}\delta_{\varphi^i,\psi^i-1}, \qquad \underline{\alpha} = \overline{1, s},$$

where $\delta_{i,j}$ is Kronecker delta.

Master equation for the state vector φ^i

$$\frac{\partial p(\varphi^i, t)}{\partial t} = \sum_{\underline{\alpha}=1}^{s} \Big\{ {}^{-}s_{\underline{\alpha}}(\varphi^i + r^{i\underline{\alpha}}, t) p(\varphi^i + r^{i\underline{\alpha}}, t) + \\ + {}^{+}s_{\underline{\alpha}}(\varphi^i - r^{i\underline{\alpha}}, t) p(\varphi^i - r^{i\underline{\alpha}}, t) - \\ - \Big[{}^{+}s_{\underline{\alpha}}(\varphi^i) + {}^{-}s_{\underline{\alpha}}(\varphi^i) \Big] p(\varphi^i, t) \Big\}.$$

The transition probabilities for master equation

$$
{}^{+}s_{\underline{\alpha}} = {}^{+}k_{\underline{\alpha}} \prod_{\underline{i}=1}^{n} A_{\varphi^{\underline{i}}}^{I^{\underline{i}\underline{\alpha}}} = {}^{+}k_{\underline{\alpha}} \prod_{\underline{i}=1}^{n} \frac{\varphi^{\underline{i}}!}{(\varphi^{\underline{i}} - I^{\underline{i}\underline{\alpha}})!},
$$

$$
{}^{-}s_{\underline{\alpha}} = {}^{-}k_{\underline{\alpha}} \prod_{\underline{i}=1}^{n} A_{\varphi^{\underline{i}}}^{F^{\underline{i}\underline{\alpha}}} = {}^{-}k_{\underline{\alpha}} \prod_{\underline{i}=1}^{n} \frac{\varphi^{\underline{i}}!}{(\varphi^{\underline{i}} - F^{\underline{i}\underline{\alpha}})!}.
$$

The transition probabilities for Fokker–Planck equation

$$\overset{+}{\underset{\mathrm{fp}}{}}s_{\underline{\alpha}} = {}^{+}k_{\underline{\alpha}} \prod_{\underline{i}=1}^{n} (\varphi^{\underline{i}})^{I^{\underline{i\alpha}}},$$

$$\overset{-}{\underset{\mathrm{fp}}{}}s_{\underline{\alpha}} = {}^{-}k_{\underline{\alpha}} \prod_{\underline{i}=1}^{n} (\varphi^{\underline{i}})^{F^{\underline{i\alpha}}}.$$

Fokker–Planck equation

$$\frac{\partial p(\varphi, t)}{\partial t} = -\frac{\partial}{\partial \varphi}\left[A(\varphi)p(\varphi, t)\right] + \frac{\partial^2}{\partial \varphi^2}\left[B(\varphi)p(\varphi, t)\right],$$

Multidimensional Fokker–Planck equation

$$\frac{\partial p(\varphi^k, t)}{\partial t} = -\frac{\partial}{\partial \varphi^i}\left[A^i(\varphi^k)p(\varphi^k, t)\right] + \\ + \frac{1}{2}\frac{\partial^2}{\partial \varphi^i \partial \varphi^j}\left[B^{ij}(\varphi^k)p(\varphi^k, t)\right],$$

where

$$A^i := A^i(\varphi^k) = r^{i\underline{\alpha}}\left[\overset{+}{\text{fp}}s_{\underline{\alpha}} - \overset{-}{\text{fp}}s_{\underline{\alpha}}\right],$$

$$B^{ij} := B^{ij}(\varphi^k) = r^{i\underline{\alpha}}r^{j\underline{\alpha}}\left[\overset{+}{\text{fp}}s_{\underline{\alpha}} - \overset{-}{\text{fp}}s_{\underline{\alpha}}\right].$$

Langevin equation

$$\mathrm{d}\varphi^i = a^i \,\mathrm{d}t + b^i_a \,\mathrm{d}W^a \,,$$

where $a^i := a^i(\varphi^k)$, $b^i_a := b^i_a(\varphi^k)$, $\varphi^i \in \mathfrak{R}^n$ is the system state vector, $W^a \in \mathbb{R}^m$ is the m-dimensional Wiener process.

The connection between the Fokker–Planck equation and Langevin equation

$$A^i = a^i, \qquad B^{ij} = b^i_a b^{ja}.$$

Occupation number representation

- It is possible to consider systems with a variable number of particles (non-stationary systems).
- System statistics (Fermi–Dirac or Bose–Einstein) is automatically included in the commutation rules for the creation and annihilation operators.
- This is the second major formalism (along with the path integral) for the quantum perturbation theory description.

Dirac notation

$$\varphi_i^* := \varphi_i = (\varphi^i)^\dagger \equiv \langle i| = |i\rangle^\dagger .$$

The scalar product

$$\varphi_i \varphi^i \equiv \langle i|i\rangle .$$

The tensor product

$$\varphi_j \varphi^i \equiv |i\rangle \langle j| .$$

Components

$$|\varphi\rangle \equiv \varphi^{i}, \qquad \langle \underline{i}|\varphi\rangle \equiv \varphi^{i}\delta^{\underline{i}}_{i} = \varphi^{\underline{i}}.$$

Linear operator

$$A^{i}_{j}\varphi_{i}\psi^{j} \equiv \langle\varphi|A|\psi\rangle .$$

$$A^{\underline{i}}_{\underline{j}} = A^{i}_{j}\delta^{\underline{i}}_{i}\delta^{j}_{\underline{j}} \equiv \langle\underline{i}|A|\underline{j}\rangle .$$

State vector

$$\varphi_n := p_n(\varphi, t).$$

Scalar product

$$\langle \varphi | \psi \rangle_{\text{ex}} = \sum_n n! p_n^*(\varphi) p^n(\psi);$$

$$\langle \varphi | \psi \rangle_{\text{in}} = \sum_n \frac{1}{k!} n_k^*(\varphi) n^k(\psi).$$

Factorial moments

$$n_k(\varphi) = \langle n(n-1)\cdots(n-k+1)\rangle = \frac{\partial^k}{\partial z^k} G(z,\varphi)|_{z=1},$$

Generating function

$$G(z,\varphi) = \sum_n z^n p_n(\phi).$$

$$\sum_n p_n(\varphi) = 1, \qquad G(1,\varphi) = 1, \qquad n_0(\varphi) = 1.$$

Normalization

$$\langle n|m\rangle_{\text{ex}} = n!\delta_n^m.$$

$$\varphi_n = \frac{1}{n!}\langle n|\varphi\rangle_{\text{ex}}.$$

Creation and annihilation operators

$$\pi \left| n \right\rangle = \left| n+1 \right\rangle ,$$
$$a \left| n \right\rangle = n \left| n-1 \right\rangle$$

with commutation rule:

$$[a, \pi] = 1.$$

Liouville equation

$$\frac{\partial}{\partial t} \left|\varphi(t)\right\rangle = L \left|\varphi(t)\right\rangle .$$

Single Liouville equation and the master equations

$$\frac{\partial p_n}{\partial t} = \frac{1}{n!} \left\langle n \middle| \frac{\partial}{\partial t} \middle| \varphi \right\rangle = \frac{1}{n!} \left\langle n | L | \varphi \right\rangle \equiv \sum_m [w_{nm} p_m - w_{mn} p_n],$$

Liouville operator

$$L = \sum_{\underline{\alpha},\underline{i}} \Big[{}^{+}k_{\underline{\alpha}} \Big((\pi_{\underline{i}})^{F^{i\alpha}_{\underline{}}} - (\pi_{\underline{i}})^{I^{i\alpha}_{\underline{}}} \Big) (a_{\underline{i}})^{I^{i\alpha}_{\underline{}}} + \\ + {}^{-}k_{\underline{\alpha}} \Big((\pi_{\underline{i}})^{I^{i\alpha}_{\underline{}}} - (\pi_{\underline{i}})^{F^{i\alpha}_{\underline{}}} \Big) (a_{\underline{i}})^{F^{i\alpha}_{\underline{}}} \Big].$$

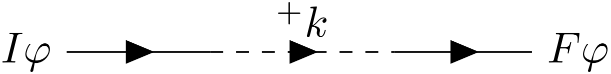

Figure 5. Forward interaction

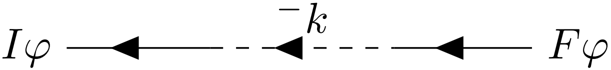

Figure 6. Backward interaction

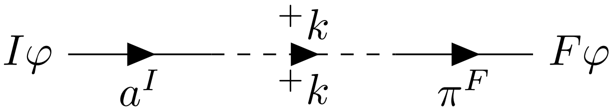

Figure 7. Forward interaction (operator approach)

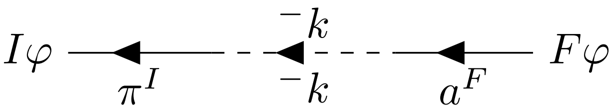

Figure 8. Backward interaction (operator approach)

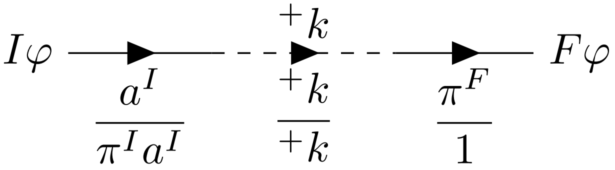

Figure 9. Forward interaction (operator approach), extended notation

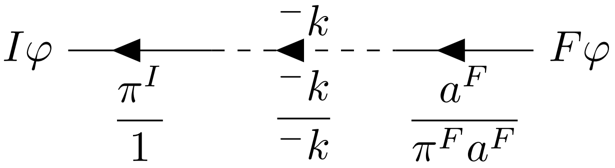

Figure 10. Backward interaction (operator approach), extended notation

We obtain a factor ${}^{+}k\pi^{F}a^{I}$. However, this violates the equation:

$$\langle 0| L = 0.$$

Redressing this, we have to subtract the number of entities that have entered into interaction, multiplied by the intensity of the interaction. Then we get a following term of the Liouville operator:

$${}^{+}k\pi^{F}a^{I} - {}^{+}k\pi^{I}a^{I} = {}^{+}k\left(\pi^{F} - \pi^{I}\right)a^{I}.$$

The general form of the master equation for the state vector φ^i, changing by steps with length $r^{i\underline{\alpha}}$, is:

$$\frac{\partial p(\varphi^i,t)}{\partial t} = \sum_{\underline{\alpha}=1}^{s} \Big\{ {}^{-}s_{\underline{\alpha}}(\varphi^i + r^{i\underline{\alpha}}, t) p(\varphi^i + r^{i\underline{\alpha}}, t) + \\ + {}^{+}s_{\underline{\alpha}}(\varphi^i - r^{i\underline{\alpha}}, t) p(\varphi^i - r^{i\underline{\alpha}}, t) - \Big[{}^{+}s_{\underline{\alpha}}(\varphi^i) + {}^{-}s_{\underline{\alpha}}(\varphi^i) \Big] p(\varphi^i, t) \Big\}.$$

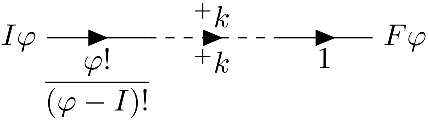

Figure 11. Forward interaction (combinatorial approach)

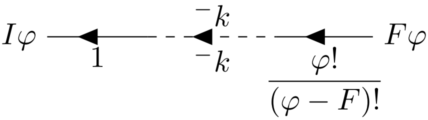

Figure 12. Backward interaction (combinatorial approach)

$$
\begin{aligned}
{}^{+}s(\varphi) &= {}^{+}k \frac{\varphi!}{(\varphi - I)!}, \\
{}^{-}s(\varphi) &= {}^{-}k \frac{\varphi!}{(\varphi - F)!}.
\end{aligned}
$$

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = \lambda\varphi - \beta\varphi - \gamma\varphi^2,$$

where λ denotes the breeding intensity factor, β — the extinction intensity factor, γ — the factor of population reduction rate.

The interaction scheme:

$$\varphi \underset{\gamma}{\overset{\lambda}{\rightleftharpoons}} 2\varphi,$$

$$\varphi \xrightarrow{\beta} 0.$$

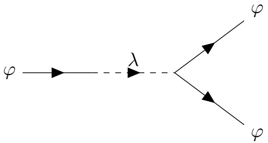

Figure 13. First forward interaction

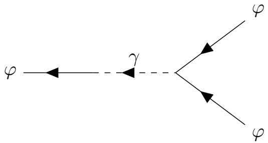

Figure 14. First backward interaction

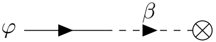

Figure 15. Second forward interaction

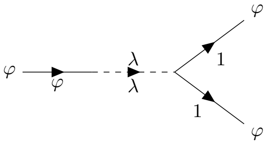

Figure 16. First forward interaction (combinatorial approach)

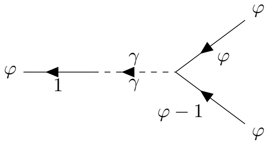

Figure 17. First backward interaction (combinatorial approach)

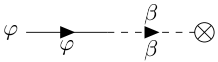

Figure 18. Second forward interaction (combinatorial approach)

Let's define transition rates within the Verhults model as follows:

$$
\begin{aligned}
{}^{+}s_1(\varphi) &= \lambda\varphi, & {}^{+}s_1(\varphi-1) &= \lambda(\varphi-1), & {}^{+}s_1(\varphi+1) &= \lambda(\varphi+1),\\
{}^{-}s_1(\varphi) &= \gamma\varphi(\varphi-1), & {}^{-}s_1(\varphi-1) &= \gamma(\varphi-1)(\varphi-2), & {}^{-}s_1(\varphi+1) &= \gamma(\varphi+1)\varphi,\\
{}^{+}s_2(\varphi) &= \beta\varphi. & {}^{+}s_2(\varphi-1) &= \beta(\varphi-1). & {}^{+}s_2(\varphi+1) &= \beta(\varphi+1).
\end{aligned}
$$

$$
r^1 = 1, \qquad r^2 = -1.
$$

Then the form of the master equation is:

$$\frac{\partial p(\varphi,t)}{\partial t} = -[\lambda\varphi + \beta\varphi + \gamma\varphi(\varphi-1)]p(\varphi,t) + \\ + [\beta(\varphi+1) + \gamma(\varphi+1)\varphi]p(\varphi+1,t) + \lambda(\varphi-1)p(\varphi-1,t).$$

For particular values of φ:

$$\frac{\partial p_n(t)}{\partial t} := \frac{\partial p(\varphi,t)}{\partial t}\bigg|_{\varphi=n} = -[\lambda n + \beta n + \gamma n(n-1)]p_n(t) + \\ + [\beta(n+1) + \gamma(n+1)n]p_{n+1}(t) + \lambda(n-1)p_{n-1}(t).$$

$$\frac{\partial}{\partial t}\left|\varphi(t)\right\rangle = L\left|\varphi(t)\right\rangle.$$

The Liouville equation in the form of a single equation writes down the master equations for different values of n.

$$\frac{\partial p_n}{\partial t} = \frac{1}{n!}\left\langle n\middle|\frac{\partial}{\partial t}\middle|\varphi\right\rangle = \frac{1}{n!}\left\langle n|L|\varphi\right\rangle \equiv \sum_m [w_{nm}p_m - w_{mn}p_n],$$

Generic Liouville operator:

$$L = \sum_{\underline{\alpha},\underline{i}}\left[{}^{+}k_{\underline{\alpha}}\left((\pi_{\underline{i}})^{F^{\underline{i\alpha}}} - (\pi_{\underline{i}})^{I^{\underline{i\alpha}}}\right)(a_{\underline{i}})^{I^{\underline{i\alpha}}} + {}^{-}k_{\underline{\alpha}}\left((\pi_{\underline{i}})^{I^{\underline{i\alpha}}} - (\pi_{\underline{i}})^{F^{\underline{i\alpha}}}\right)(a_{\underline{i}})^{F^{\underline{i\alpha}}}\right].$$

The Liouville operator is:

$$
\begin{aligned}
L = \lambda(\pi^2 - \pi)a + \gamma(\pi - \pi^2)a^2 + \beta(1 - \pi)a = \\
= \lambda\Big((a^\dagger)^2 - a^\dagger\Big)a + \gamma\Big(a^\dagger - (a^\dagger)^2\Big)a^2 + \beta\Big(1 - a^\dagger\Big)a = \\
= \lambda\Big(a^\dagger - 1\Big)a^\dagger a + \beta\Big(1 - a^\dagger\Big)a + \gamma\Big(1 - a^\dagger\Big)a^\dagger a^2.
\end{aligned}
$$

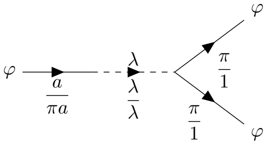

Figure 19. First forward interaction (operator approach)

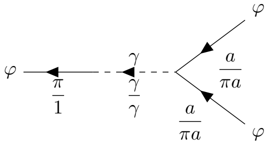

Figure 20. First backward interaction (operator approach)

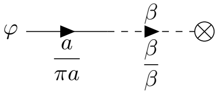

Figure 21. Second forward interaction (operator approach)

The master equation by Liouville operator:

$$
\begin{aligned}
\frac{\partial p_n(t)}{\partial t} = \frac{1}{n!} \langle n| L |\varphi\rangle = \frac{1}{n!} \langle n| - \left[\lambda a^\dagger a + \beta a^\dagger a + \gamma a^\dagger a^\dagger a a\right] + \\
+ \left[\beta a + \gamma a^\dagger a a\right] + \lambda a^\dagger a^\dagger a |\varphi\rangle = \\
= -[\lambda n + \beta n + \gamma n(n-1)] \langle n|\varphi\rangle + \\
+ [\beta(n+1) + \gamma(n+1)n] \langle n+1|\varphi\rangle + \lambda(n-1) \langle n-1|\varphi\rangle = \\
= -[\lambda n + \beta n + \gamma n(n-1)] p_n(t) + \\
+ [\beta(n+1) + \gamma(n+1)n] p_{n+1}(t) + \lambda(n-1) p_{n-1}(t).
\end{aligned}
$$

The result coincides with the formula, which was obtained by combinatorial method.