Part I
The generating function

The generating function is a mathematical tool, often used as a method to easily derive the elements of a series. Let's look at a simple example.

1 The Fibonacci's series

The Fibonacci's series is defined by:

$$F_{n+1} = F_n + F_{n-1} \qquad (n \geq 1; F_0 = 0; F_1 = 1). \tag{1}$$

Obviously, one can generate any term of the series in a sequential manner. However, defining a generating function can simplify the process of generating the series elements. Let's define,

$$F(x) \equiv \sum_{n=1}^{\infty} x^n F_n. \tag{2}$$

Multiplying the equation defining the Fibonacci's series (eq. 1) by x^n and summing over n yields,

$$\sum_{n=1}^{\infty} x^n F_{n+1} = \sum_{n=1}^{\infty} x^n F_n + \sum_{n=1}^{\infty} x^n F_{n-1}. \tag{3}$$

We can rewrite the LHS as:

$$\sum_{n=1}^{\infty} x^n F_{n+1} = \frac{1}{x}\sum_{n=1}^{\infty} x^{n+1} F_{n+1} = \frac{1}{x}\left(\sum_{n=0}^{\infty} x^{n+1} F_{n+1} - xF_1\right) = \frac{1}{x}\left(\sum_{n=1}^{\infty} x^n F_n - x\right) = \frac{F(x)}{x} - 1. \tag{4}$$

The RHS may be written as:

$$\sum_{n=1}^{\infty} x^n F_n + \sum_{n=1}^{\infty} x^n F_{n-1} = F(x) + x\sum_{n=1}^{\infty} x^{n-1} F_{n-1} = F(x) + x\sum_{n=1}^{\infty} x^n F_n = (1+x)F(x). \tag{5}$$

Note that in the change from $n-1$ to n, we dropped the $n = 0$ term because it is zero. Equation (3) may be written as:

$$\frac{F(x)}{x} - 1 = (1+x)F(x) \tag{6}$$
$$F(x) = -\frac{x}{x + x^2 - 1} = \frac{x}{1 - x - x^2}.$$

The $n'th$ derivative of $F(x)$ (with respect to x) at $x = 0$ divided by $n!$ is the $n'th$ term of the Fibonacci's series. In this case, it's possible to derive an exact formula for the series terms. Let's write the generating function using partial fractions

$$F(x) = \frac{x}{1-x-x^2} = \frac{1}{(r_+ - r_-)}\left(\frac{1}{1-xr_+} - \frac{1}{1-xr_-}\right) \qquad r_\pm = \left(1 \pm \sqrt{5}\right)/2. \tag{7}$$

Using the sum of the geometric series one may write it as:

$$F(x) = \frac{1}{(r_+ - r_-)}\left(\sum_{n=0}^{\infty} r_+^n x^n - \sum_{n=0}^{\infty} r_-^n x^n\right) = \frac{1}{\sqrt{5}}\sum_{n=0}^{\infty}\left(r_+^n - r_-^n\right) x^n. \tag{8}$$

The use of the sum is legitimate because we are interested in the function near $x \to 0$. The $n'th$ Fibonacci's term is simply

$$F_n = \frac{1}{\sqrt{5}}\left(r_+^n - r_-^n\right). \tag{9}$$

2 Photon emission

The generating function is a very useful tool in counting statistics. One of the simplest examples of counting statistics is the photon emission counting statistics from a two level system (TLS) driven by an external field. A schematic description of the system is provided below. The system consists of two electronic levels, excited (e) and ground (g) states. The external field excites the system from the ground state to the excited state with a rate k and the system relaxes to the ground state through the spontaneous emission of a photon with a rate Γ. If one is only interested in the TLS, there are only two states and the Master equation describing the dynamics is easily written as:

$$\frac{d}{dt}\begin{pmatrix} P_g(t) \\ P_e(t) \end{pmatrix} = \begin{pmatrix} -k & \Gamma \\ k & -\Gamma \end{pmatrix}\begin{pmatrix} P_g(t) \\ P_e(t) \end{pmatrix} \tag{10}$$

Here, $P_{g,e}(t)$ is the probability to find the system in the g, e state, at time t. However, this equation does not allow to track the emission of photons. In order to gain information regarding the photon statistics one has to extend the states of the system to include both the electronic state and the number of photons previously emitted (as shown in the figure below).

When the information regarding the number of emitted photons is included, there is an infinite number of states and the dynamics is described by the infinite Master equation:

$$\begin{aligned} \frac{d}{dt}P_{g,n}(t) &= -kP_{g,n}(t) + \Gamma P_{e,n-1}(t); \\ \frac{d}{dt}P_{e,n}(t) &= kP_{g,n}(t) - \Gamma P_{e,n}(t). \end{aligned} \tag{11}$$

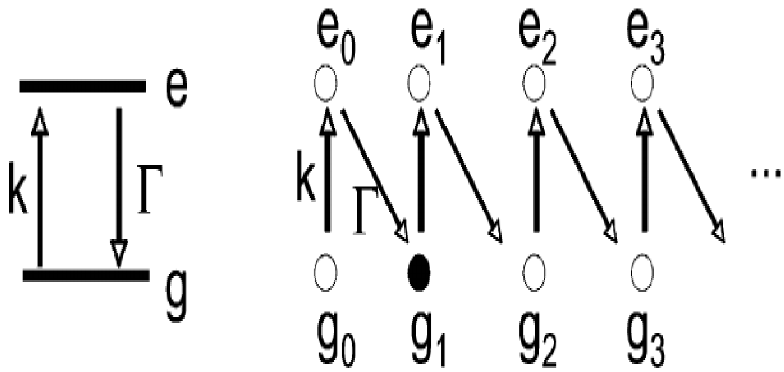


Figure 1: (Left) Schematic description of the TLS and the excitation and relaxation processes. (Right) Schematic description of the process with states accounting for electronic state and for the number of photons previously emitted by the TLS.

We define the generating functions as:

$$G_g(s,t) = \sum_{n=0}^{\infty} P_{g,n}(t)\, s^n; \tag{12}$$
$$G_e(s,t) = \sum_{n=0}^{\infty} P_{e,n}(t)\, s^n.$$

Multiplying the Master equation (11) by s^n and summing over n yield the equations describing the dynamics of the generating functions.

$$\frac{d}{dt}\begin{pmatrix} G_g(s,t) \\ G_e(s,t) \end{pmatrix} = \begin{pmatrix} -k & s\Gamma \\ k & -\Gamma \end{pmatrix}\begin{pmatrix} G_g(s,t) \\ G_e(s,t) \end{pmatrix} = \mathcal{M}(s)\begin{pmatrix} G_g(s,t) \\ G_e(s,t) \end{pmatrix}. \tag{13}$$

The formal solution is:

$$\begin{pmatrix} G_g(s,t) \\ G_e(s,t) \end{pmatrix} = \exp\left(\mathcal{M}(s)\, t\right)\begin{pmatrix} G_g(s,0) \\ G_e(s,0) \end{pmatrix}. \tag{14}$$

If one is only interested in the number of photons emitted (which is measurable in experiments) and not in the state of the system, the corresponding generating function is $G(s,t) = G_g(s,t) + G_e(s,t)$ (namely we sum the probabilities of being in the ground and excited states after emitting n photons). The photon counting moments are given by,

$$\frac{\partial^m}{\partial s^m} G(s,t)\,|_{s=1} = \langle n(n-1)\,..\,(n-m+1)\rangle\,. \tag{15}$$

The matrix $\mathcal{M}$ is diagonalizable, thereby allowing analytical solution of the equation for the generating function. Assuming that the system is initially in the ground state one obtains the following generating function,

$$G(s,t) = \frac{e^{-[(\Gamma+k-f(s))t/2]}\left(\Gamma+k+f(s)\right) - e^{-[(\Gamma+k+f(s))t/2]}\left(\Gamma+k-f(s)\right)}{2f(s)}, \tag{16}$$

$$f(s) = \sqrt{(\Gamma-k)^2 + 4sk\Gamma}.$$

The emission rate is

$$I = \lim_{t\to\infty}\frac{\partial\langle n\rangle}{\partial t} = \lim_{t\to\infty}\frac{\partial}{\partial t}\left(\frac{\partial G(s,t)}{\partial s}|_{s=1}\right) = \frac{\Gamma k}{k+\Gamma}.$$

And the Q parameter is

$$Q = \lim_{t\to\infty}\frac{\langle n^2\rangle - \langle n\rangle^2}{\langle n\rangle} - 1 = \lim_{t\to\infty}\frac{\frac{\partial^2 G(s,t)}{\partial s^2}|_{s=1} - \left(\frac{\partial G(s,t)}{\partial s}|_{s=1}\right)^2}{\frac{\partial G(s,t)}{\partial s}|_{s=1}} = -\frac{2\Gamma k}{(k+\Gamma)^2}.$$

Note that the negative value of the Q parameter indicates the sub-Poissonian statistics of the number of photons.

For Poissonian distribution we have

$$P(n) = \frac{\lambda^n}{n!}e^{-\lambda}$$

Therefore,

$$\langle n\rangle = \sum_{n=0}^{\infty} n\frac{\lambda^n}{n!}e^{-\lambda} = \sum_{n=1}^{\infty}\frac{\lambda^n}{(n-1)!}e^{-\lambda} = \lambda\sum_{n=1}^{\infty}\frac{\lambda^{n-1}}{(n-1)!}e^{-\lambda} = \lambda\sum_{n=0}^{\infty}\frac{\lambda^n}{n!}e^{-\lambda} = \lambda$$

$$\langle n^2\rangle = \sum_{n=0}^{\infty} n^2\frac{\lambda^n}{n!}e^{-\lambda} = \sum_{n=0}^{\infty}\left(n(n-1)+n\right)\frac{\lambda^n}{n!}e^{-\lambda} = \langle n\rangle + \lambda^2\sum_{n=2}^{\infty}\frac{\lambda^{n-2}}{(n-2)!}e^{-\lambda} = \langle n\rangle + \lambda^2$$

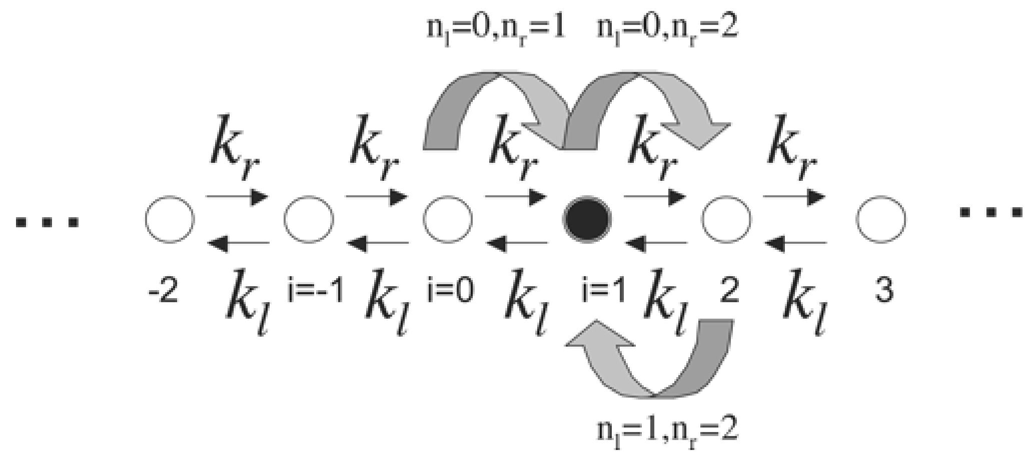
and

$$Q_{Poissonian} = \frac{\langle n^2\rangle - \langle n\rangle^2}{\langle n\rangle} - 1 = \frac{\langle n\rangle + \lambda^2 - \lambda^2}{\langle n\rangle} - 1 = 0.$$

3 1D Random Walk

The next example is somewhat more complicated because we need to count two types of events. We consider a version of one of the fundamental problems in statistical physics, the random walk in 1d.

Consider a random walker that takes steps to the left with a rate k_l and steps to the right with a rate k_r.



Schematic description of the 1D random walk.

One of the methods to describe the process is to consider the probability that the walker completed n_r steps to the right and n_l steps to the left by time t. We denote this probability by $p_{n_l,n_r}(t)$. Let's consider the dynamics of the probability that by time t the walker haven't made any jump. From the no jump state the walker can move either to the state of 1 jump to the left ($n_l = 1, n_r = 0$) or to the state of 1 jump to the right ($n_l = 0, n_r = 1$). The equation describing this dynamics takes the form

$$\frac{d}{dt}p_{n_l=0,n_r=0}(t) = -(k_l + k_r)\,p_{n_l=0,n_r=0}(t)\,. \tag{17}$$

Similarly we can write for the probabilities that by time t the walker made 1 step to the right/left

$$\begin{aligned}\frac{d}{dt}p_{n_l=1,n_r=0}(t) &= -(k_l + k_r)\,p_{n_l=1,n_r=0}(t) + k_l p_{n_l=0,n_r=0}(t)\,; \\ \frac{d}{dt}p_{n_l=0,n_r=1}(t) &= -(k_l + k_r)\,p_{n_l=0,n_r=1}(t) + k_r p_{n_l=0,n_r=0}(t)\,.\end{aligned} \tag{18}$$

In general, the infinite master equation describing the dynamics of the probabilities that n_r, n_l hops to the right,left have occurred by time t is:

$$\frac{d}{dt}p_{n_l,n_r}(t) = -(k_l + k_r)\,p_{n_l,n_r}(t) + k_r p_{n_l,n_r-1}(t) + k_l p_{n_l-1,n_r}(t)\,. \tag{19}$$

The position of the particle, relative to the initial position, is given by $n_r - n_l$.

In order to fully characterize the dynamics one has to know either all the probabilities or equivalently all the moments– $\langle n_l^m n_r^q \rangle$. In order to find all the moments we define the generating function:

$$G\left(s_l, s_r, t\right) \equiv \sum_{n_l, n_r=0}^{\infty} p_{n_l, n_r}\left(t\right) s_l^{n_l} s_r^{n_r}, \tag{20}$$

s_l, s_r are two auxiliary variables that will be used to derive the statistics of the random walker.

From the definition in eq. (20) we can extract the probability by differentiating the generating function and evaluating at $s_l = s_r = 0$.

$$p_{m_l, m_r}\left(t\right) = \frac{1}{m_l! m_r!} \frac{\partial^{m_l} \partial^{m_r}}{\partial s_l^{m_l} \partial s_r^{m_r}} G\left(s_l, s_r, t\right)|_{s_l=s_r=0}. \tag{21}$$

The moments of the number of jumps are given by,

$$\left\langle n_l\left(n_l-1\right) \ldots\left(n_l-a+1\right) n_r\left(n_r-1\right) \ldots\left(n_r-b+1\right)\right\rangle(t) = \frac{\partial^a \partial^b}{\partial s_l^a \partial s_r^b} G\left(s_l, s_r, t\right)|_{s_l=s_r=1}. \tag{22}$$

The equation of motion for the generating function is obtained by multiplying eq. (19) by $s_l^{n_l} s_r^{n_r}$ and summing over all non-negative integer values of n_r and n_l. The equation reads:

$$\frac{\partial}{\partial t} G\left(s_l, s_r, t\right) = \left[-\left(k_l+k_r\right)+k_r s_r+k_l s_l\right] G\left(s_l, s_r, t\right). \tag{23}$$

The solution to this equation is (assuming that at $t=0$, $n_r = n_l = 0$).

$$G\left(s_l, s_r, t\right) = e^{-k_r\left(1-s_r\right) t} e^{-k_l\left(1-s_l\right) t}. \tag{24}$$

The joint probability distribution for left and right jumps reflects two statistically independent Poisson distributions. Applying the formula of eq. (21) to the expression for the generating function in eq. (24) yields,

$$p_{m_l, m_r}\left(t\right) = \frac{1}{m_l!}\left(k_l t\right)^{m_l} e^{-k_l t} \frac{1}{m_r!}\left(k_r t\right)^{m_r} e^{-k_r t}. \tag{25}$$

The probability to find the walker at site i at time t is given by

$$\begin{aligned} P_i\left(t\right) &= \sum_{n_l, n_r=0}^{\infty} p_{n_l, n_r}\left(t\right) \delta_{n_r-n_l, i} = \sum_{m_l, m_r=0}^{\infty} \frac{1}{m_l!}\left(k_l t\right)^{m_l} e^{-k_l t} \frac{1}{m_r!}\left(k_r t\right)^{m_r} e^{-k_r t} \delta_{m_r-m_l, i} \\ &= e^{-\left(k_l+k_r\right) t} \sum_{m_l}^{\infty}{}' \frac{\left(k_l t\right)^{m_l}}{m_l!} \frac{\left(k_r t\right)^{m_l+i}}{\left(m_l+i\right)!}, \end{aligned} \tag{26}$$

where the $'$ denotes that the sum is only over non-negative values of $m_l + i$ and m_l.

Using eq. (22) we find

$$\langle n_l \rangle = \frac{\partial}{\partial s_l} G(s_l, s_r, t)|_{s_l=s_r=1} = k_l t; \tag{27}$$

$$\langle n_r \rangle = \frac{\partial}{\partial s_r} G(s_l, s_r, t)|_{s_l=s_r=1} = k_r t; \tag{28}$$

$$\langle i \rangle = \langle n_r \rangle - \langle n_l \rangle = (k_r - k_l)\, t. \tag{29}$$

Similarly we derive the second moments

$$\left\langle n_l^2 - n_l \right\rangle = \frac{\partial^2}{\partial s_l^2} G(s_l, s_r, t)|_{s_l=s_r=1} = (k_l t)^2; \tag{30}$$

$$\left\langle n_r^2 - n_r \right\rangle = \frac{\partial^2}{\partial s_r^2} G(s_l, s_r, t)|_{s_l=s_r=1} = (k_r t)^2; \tag{31}$$

$$\langle n_r n_l \rangle = \frac{\partial^2}{\partial s_r \partial s_l} G(s_l, s_r, t)|_{s_l=s_r=1} = (k_l t)(k_r t); \tag{32}$$

$$\begin{aligned} \left\langle i^2 \right\rangle - \langle i \rangle^2 &= \left\langle n_r^2 \right\rangle + \left\langle n_l^2 \right\rangle - 2\langle n_l n_r \rangle - \langle n_r \rangle^2 - \langle n_l \rangle^2 + 2\langle n_r \rangle \langle n_l \rangle \\ &= (k_r + k_l)\, t; \end{aligned} \tag{33}$$

In the limit of $t \to \infty$ the probability density function of i is well approximated by

$$P_i(t) \approx \frac{1}{\sqrt{2\pi (k_r + k_l)\, t}} e^{-\frac{(i-(k_r-k_l)t)^2}{2(k_r+k_l)t}}. \tag{34}$$

We showed here that the generating function helps to reduce an infinite set of coupled equations to a finite number of equations. The dynamics of the generating function is easily derived from the original equations of motion. The statistics of the process is easily derived by differentiating the generating function. The generating function can be used to track multiple types of events.

The continuous description of the random walk is well approximated at the long time limit by the diffusion equation. The diffusion describes the probability in the ensemble sense. In the model we considered above, the rate of jumping left is k_l, and the rate of jumping right is k_r. Therefore, the probability that a jump occurred up to time τ is given by

$$P_{jump}(\tau) = \int_0^\tau k e^{-kt'} dt' = 1 - e^{-k\tau}. \tag{35}$$

Here, we define $k \equiv k_l + k_r$. For later use we also define $\varepsilon \equiv \frac{k_r - k_l}{k}$. The probability to jump to the left/right, up to time τ is then $P_{jumpl,jumpr}(\tau) = \frac{k_{l,r}}{k} P_{jump}(\tau)$, correspondingly.

************************* A comment regarding the jump rate

The cumulative distribution for the time to jump left is

$$P_l\left(\tau\right)=\int\limits_0^\tau k_l e^{-k_l t'}dt'=1-e^{-k_l\tau}.$$

Therefore, the probability that the time for the jump to the left is larger than t is given by

$$W\left(\tau_l>t\right)=1-P_l\left(t\right)=e^{-k_l t}.$$

Similarly,

$$W\left(\tau_r>t\right)=1-P_r\left(t\right)=e^{-k_r t}.$$

Our basic assumption is that the jumps to the left and to the right are independent, and therefore,

$$W\left(\tau_l>t,\tau_r>t\right)=W\left(\tau_r>t\right)W\left(\tau_l>t\right)=e^{-(k_l+k_r)t}.$$

The PDF of $Z=\min\left(\tau_r,\tau_l\right)$ is

$$p(Z)=-\frac{dW\left(\tau_l>t,\tau_r>t\right)}{dt}|_{t=Z}=\left(k_l+k_r\right)e^{-(k_l+k_r)Z}$$

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If we consider a forward step in time, from time $t-\tau$ to time t, then, since the probability is conserved, we obtain for the probability density at position x the following relation:

$$\begin{aligned}p(x,t)=&\,p\left(x,t-\tau\right)\left(1-P_{jump}\left(\tau\right)\right)\\&+p\left(x-a,t-\tau\right)P_{jumpr}\left(\tau\right)+p\left(x+a,t-\tau\right)P_{jumpl}\left(\tau\right)\end{aligned}\tag{36}$$

The first term in the RHS describes the probability that the walker was at position x at time $t-\tau$ and hasn't moved. The second term describes the gained probability due to walkers at position $x-a$, at time $t-\tau$ and similarly, the third term describes the gained probability due to walkers at position $x+a$, at time $t-\tau$. Expanding the above expression in a Taylor series we obtain:

$$\begin{aligned}p(x,t)=&\left(p(x,t)-\tau\frac{\partial p\left(x,t\right)}{\partial t}\right)\left(1-P_{jump}\left(\tau\right)\right)\\&+\left(p(x,t)-\tau\frac{\partial p\left(x,t\right)}{\partial t}-a\frac{\partial p\left(x,t\right)}{\partial x}+\frac{1}{2}a^2\frac{\partial^2 p\left(x,t\right)}{\partial x^2}\right)P_{jumpr}\left(\tau\right)\\&+\left(p(x,t)-\tau\frac{\partial p\left(x,t\right)}{\partial t}+a\frac{\partial p\left(x,t\right)}{\partial x}+\frac{1}{2}a^2\frac{\partial^2 p\left(x,t\right)}{\partial x^2}\right)P_{jumpl}\left(\tau\right)\\&+O\left(\tau^2\right)+O\left(a^3\right)+O\left(a\tau\right)\end{aligned}\tag{37}$$

Rearranging the terms we obtain:

$$\begin{aligned}\frac{\partial p(x,t)}{\partial t} &= \frac{a}{\tau}\left(P_{jumpl}(\tau)-P_{jumpr}(\tau)\right)\frac{\partial p(x,t)}{\partial x} \\ &+ \frac{a^2}{2\tau}\left(P_{jumpr}(\tau)+P_{jumpl}(\tau)\right)\frac{\partial^2 p(x,t)}{\partial x^2} \\ &+ O\left(\tau^2\right)+O\left(a^3\right)+O\left(a\tau\right).\end{aligned} \tag{38}$$

Defining

$$\begin{aligned}D &\equiv \lim_{a,\tau\to 0}\frac{\left(P_{jumpr}(\tau)+P_{jumpl}(\tau)\right)a^2}{2\tau} = \frac{\left(k_l+k_r\right)a^2}{2} = \frac{ka^2}{2}; \\ u &\equiv \lim_{a,\tau,\varepsilon\to 0}\frac{\left(P_{jumpl}(\tau)-P_{jumpr}(\tau)\right)a}{\tau} = \left(k_r-k_l\right)a = \frac{2\left(k_l-k_r\right)}{ak}\frac{ka^2}{2} = 2\frac{\varepsilon}{a}D.\end{aligned} \tag{39}$$

Using the definitions above, and neglecting higher order terms we obtain the diffusion equation

$$\frac{\partial p(x,t)}{\partial t} = -u\frac{\partial p(x,t)}{\partial x} + D\frac{\partial^2 p(x,t)}{\partial x^2}. \tag{40}$$

It is possible to solve the equation for a given initial condition. It is also possible to take the generating function approach to calculate the various moments. To do that, we consider the Fourier transform of the equation

$$\widetilde{p}(q,t) = \int_{-\infty}^{\infty} e^{-iqx}p(x,t)\,dx. \tag{41}$$

Note that all the moments of x may be derived by differentiating the Fourier transform with respect to q.

$$\langle x^m\rangle = \frac{1}{(-i)^m}\frac{\partial^m\widetilde{p}(q,t)}{\partial q^m}|_{q=0}. \tag{42}$$

The Fourier transform of equation (40) reads:

$$\frac{\partial\widetilde{p}(q,t)}{\partial t} = -iqu\widetilde{p}(q,t) - Dq^2\widetilde{p}(q,t). \tag{43}$$

The solution of this equation is simple

$$\widetilde{p}(q,t) = \widetilde{p}(q,0)\,e^{-\left(iqu+Dq^2\right)t}. \tag{44}$$

A common initial condition is

$$p(x,t) = \delta(x) \to \widetilde{p}(q,0) = \int_{-\infty}^{\infty} e^{-iqx}\delta(x)\,dx = 1. \tag{45}$$

In this case, the moments are:

$$\langle x \rangle = \int_{-\infty}^{\infty} xp\left(x,t\right)dx = \frac{1}{-i}\frac{\partial \widetilde{p}\left(q,t\right)}{\partial q}|_{q=0} = ut \tag{46}$$

$$\left\langle x^2 \right\rangle = \int_{-\infty}^{\infty} x^2 p\left(x,t\right)dx = \frac{1}{\left(-i\right)^2}\frac{\partial^2 \widetilde{p}\left(q,t\right)}{\partial q^2}|_{q=0} = 2Dt + u^2 t^2 \tag{47}$$

$$\left\langle x^2 \right\rangle - \left\langle x \right\rangle^2 = 2Dt \tag{48}$$