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Quantization of Brownian Motion

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Following our work on the quantization of nonconservative systems using fractional calculus, the canonical quantization of a system with Brownian motion is carried out according to the Dirac method. A suitable Lagrangian corresponding to the Langevin equation is set up. Further, a Hamiltonian is constructed and is transformed to Schrödinger's equation which is solved.

KEY WORDS: fractional calculus; Brownian motion; nonconservative systems.

1. INTRODUCTION

The term *Brownian motion* stands for the perpetual motion of small particles immersed in fluids. The irregular motion of these particles, which are large compared to the molecules of the fluid, is caused by the very frequent impacts of the fluid molecules on them (Dass and Sharma, 1998). Einstein gave the first satisfactory theoretical treatment of this phenomenon employing statistical methods. Under the heading "Brownian motion", a wide class of physical phenomena relates properties such as the mobility of a fluid system, its coefficients of diffusion, etc., with the temperature (Pathria, 2004). The mechanism of the Brownian motion is vital in formulating, and in a certain sense solving, problems as to how "a given physical system, which is not in a state of equilibrium, finally approaches a state of equilibrium"; whereas "a physical system, which is in a state of equilibrium, persists to be in that state" (Pathria, 2004).

The quantum Brownian motion paradigm provides a unified framework where one can see the interconnection of some basic quantum statistical processes like decoherence, dissipation, particle creation, noise, and fluctuation. There were several attempts to extend the classical Langevin equation for quantum cases.

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Study of the Langevin equation for quantum systems has its origin in papers by Senitzky, Schwinger, Haken and Lax, where they investigated a quantum-mechanical damped harmonic oscillator in connection with laser systems (Kobryn *et al.*, 2003). Others noticed that the random force must be an operator defined in its own Hilbert space, which does not occur in the classical case as there is no consideration of space for the random force (Kobryn *et al.*, 2003). In all cases, scheme for the quantization of dissipative systems seems to be the stochastic quantization procedure (Hajra, 1991).

In this paper, we wish to apply our method of quantizing nonconservative, or dissipative, systems using fractional calculus (Rabei *et al.*, 2006) to quantize the Brownian motion. The paper is arranged as follows: in Section 2, we introduce the main concepts of the Brownian motion on the Langiven-equation basis. In Section 3, we introduce the main features of our method. In Section 4, the quantization of Brownian motion is carried out. This is followed by a discussion in Section 5.

2. BROWNIAN MOTION

According to the kinetic theory, fluids consist of molecules which are in incessant and random motion because of intrinsic thermal fluctuations. Hence, if there is an external particle—the Brownian particle—present in a fluid, then the molecules of the fluid, in addition to constantly colliding with each other, also collide with the Brownian particle, thereby imparting the particle with the observed random motion (Pathria, 2004). Thus, Brownian motion reveals very clearly the statistical fluctuations that occur in a system in thermal equilibrium. Historically, this phenomenon was instrumental in helping to gain the acceptance for the atomic theory of all matter and for the validity of the statistical description of physical systems.

Obviously, a Brownian particle cannot gain energy from the surrounding medium indefinitely. Therefore, a mechanism for the particle to dissipate its energy in some form so that it reaches equilibrium with the environment should exist. Early last century, Langevin suggested that the force exerted on the Brownian particle by the surrounding medium can effectively be written as a sum of two parts: (i) an "averaged out" part which represents a frictional force experienced by the particle; and (ii) a "rapidly fluctuating" part (Pathria, 2004). The "rapidly fluctuating" part, $R(t)$, is responsible for the random motion of the Brownian particle and averages out to zero over long intervals of time. The presence of the frictional force implies the existence of processes whereby the energy associated with the Brownian particle is dissipated in the course of time to the degrees of freedom corresponding to the surrounding medium. Clearly, fluctuations and dissipation have to go hand in hand if the complete system has to stay in equilibrium. Thus, we may write

$$m\frac{d\vec{v}}{dt} = -b\vec{v}(t) + \vec{R}(t), \qquad \langle\vec{R}(t)\rangle = 0. \tag{1}$$

This equation is often referred to as the *Langevin equation*. For a spherical Brownian particle of radius r moving in a fluid of viscosity η, the parameter b characterizing the dynamical friction term is given by the Stokes' formula

$$b = 6\pi r\eta. \tag{2}$$

By taking the ensemble average of Eq. (1), we obtain

$$m\frac{d}{dt}\langle\vec{v}\rangle = -b\langle\vec{v}(t)\rangle. \tag{3}$$

It follows that (Dass and Sharma, 1998; Pathria, 2004)

$$\langle v(t)\rangle = v(0)\exp\left(\frac{-t}{\tau}\right), \qquad \tau = \frac{m}{b}. \tag{4}$$

Accordingly, the drift velocity of the particle decays to zero at a rate determined by the relaxation time τ. This result is typical of dissipation phenomena such as the viscosity of the fluid; at the same time, the irreversible nature of the result is evident (Dass and Sharma, 1998; Pathria, 2004).

The instantaneous acceleration is obtained from Eq. (1):

$$\frac{d\vec{v}}{dt} = -\frac{b}{m}\vec{v}(t) + \vec{A}(t), \qquad \langle\vec{A}(t)\rangle = 0. \tag{5}$$

By constructing a scalar product of Eq. (5) with the instantaneous position $\vec{r}$, then taking the ensemble average of the product and making use of the facts

$$(i)\ \vec{r}\cdot\vec{v} = \frac{1}{2}\frac{d}{dt}r^2, \tag{6}$$

$$\text{(ii)}\ \vec{r}\cdot\frac{d}{dt}v = \frac{1}{2}\left(\frac{d^2}{dt^2}r^2\right) - v^2, \tag{7}$$

$$\text{(iii)}\ \langle\vec{r}\cdot\vec{A}\rangle = 0, \tag{8}$$

we finally obtain (Dass and Sharma, 1998; Pathria, 2004)

$$\frac{d^2}{dt^2}\langle r^2\rangle + \frac{1}{\tau}\frac{d}{dt}\langle r^2\rangle = 2\langle v^2\rangle. \tag{9}$$

For a Brownian particle in thermal equilibrium with the molecules of the fluid, the quantity $\langle v^2\rangle$ may be replaced by $3k_{\mathrm{B}}T/m$, k_{B} being Boltzmann's constant and

m the mass of the particle. Equation (9) is then solved as

$$\langle r^2 \rangle = \frac{6k_B T\tau^2}{m}\left[\frac{t}{\tau} - \left(1 - e^{-t/\tau}\right)\right]. \tag{10}$$

For $t \ll \tau$,

$$\langle r^2 \rangle \approx \frac{3k_B T t^2}{m} = \langle v^2 \rangle t^2, \tag{11}$$

which is consistent with Newton's simple equation of motion

$$\vec{r} = \vec{v}t. \tag{12}$$

For $t \gg \tau$,

$$\langle r^2 \rangle \approx \frac{6k_B T\tau}{m} = \left(\frac{6k_B T}{b}\right)t. \tag{13}$$

This is the well-known Einstein result (Dass and Sharma, 1998; Pathria, 2004). The coefficient of diffusion D is defined in terms of b as

$$D = \frac{k_B T}{b}. \tag{14}$$

3. QUANTIZATION OF NONCONSERVATIVE SYSTEMS

According to our recent theory of the quantization of nonconservative systems (Rabei *et al.*, 2006), the starting point for quantizing the Hamiltonian is to change the coordinates and momenta, $q_{r,s(i)}$ and $p_{r,s(i)}$, into operators satisfying commutation relations which correspond to the Poisson-bracket relations of the classical theory (Dirac, 1964). The first step is to connect the canonical conjugate variables, i.e., we must determine which of $p_{r,s(i)}$ and $q_{r,s(i)}$ are the canonical conjugate variables.

This canonical conjugate relation is obtained directly from Hamilton's equation defined by Riewe (1976, 1997) as follows:

$$\frac{\partial H}{\partial p_{r,s(i)}} = q_{r,s(i+1)} = \frac{d^{s(i+1)-s(i)}}{d(t-b)^{s(i+1)-s(i)}} q_{r,s(i)}, \qquad 0 \le i \le N-1. \tag{15}$$

We conclude that $p_{r,s(i)}$ is the canonical conjugate of $q_{r,s(i)}$. The Hamiltonian can then be written in the following form (Rabei *et al.*, 2006):

$$\begin{aligned} H &= \sum_{i=0}^{N-1} \frac{d^{s(i+1)-s(i)}}{d(t-b)^{s(i+1)-s(i)}} q_{r,s(i)} p_{r,s(i)} - L, \\ &= \sum_{i=0}^{N-1} q_{r,s(i+1)} p_{r,s(i)} - L, \qquad 0 \le i \le N-1 \end{aligned} \tag{16}$$

the summation rule for repeated indices being used throughout this paper. The last result, Eq. (16), is equivalent to Riewe's Hamiltonian (1976, 1997) and it is applicable to higher-order Lagrangians with integer derivatives, as obtained by Pimental and Teixeira (1997).

We define the most general classical Poisson bracket for any two functions, F and G, in phase space (Rabei *et al.*, 2006) as follows:

$$\{F, G\} = \sum_{k=0}^{N-1} \frac{\partial F}{\partial q_{r,s(k)}} \frac{\partial G}{\partial p_{r,s(k)}} - \frac{\partial F}{\partial p_{r,s(k)}} \frac{\partial G}{\partial q_{r,s(k)}}. \tag{17}$$

The fundamental Poisson brackets then read (Rabei *et al.*, 2006)

$$\begin{aligned} \left\{q_{r,s(i)}, p_{l,s(j)}\right\} = \sum_{k=0}^{N-1} & \frac{\partial q_{r,s(i)}}{\partial q_{m,s(k)}} \frac{\partial p_{l,s(j)}}{\partial p_{m,s(k)}} \\ & - \frac{\partial q_{r,s(i)}}{\partial p_{m,s(k)}} \frac{\partial p_{l,s(j)}}{\partial q_{m,s(k)}}, \qquad 0 \le i, \quad j \le N-1 \end{aligned} \tag{18}$$

$$\left\{q_{r,s(i)}, p_{l,s(j)}\right\} = \delta_{ij}\delta_{rl}. \tag{19}$$

Substituting integer derivatives, one recovers the well-known definition of Poisson brackets.

According to our definition of the Hamiltonian, Hamilton's equations of motion can be written in terms of Poisson brackets as (Rabei *et al.*, 2006)

$$\frac{d^{s(i+1)-s(i)}}{d(t-b)^{s(i+1)-s(i)}} q_{r,s(i)} = q_{r,s(i+1)} = \left\{q_{r,s(i)}, H\right\}, \tag{20}$$

and

$$(-1)^{s(i+1)-s(i)} \frac{d^{s(i+1)-s(i)}}{d(t-b)^{s(i+1)-s(i)}} p_{r,s(i)} = -\left\{p_{r,s(i)}, H\right\}. \tag{21}$$

These two definitions are valid for higher-order Lagrangians with integer derivatives and lead to the same definitions given by Pimental and Teixeira (1997). This means our definitions are more generalized than theirs; ours are applicable for fractional as well as integer systems.

We connect the canonical conjugate variables quantum-mechanically by defining the momentum operator as (Rabei *et al.*, 2006)

$$p_{s(i)} \equiv \frac{\hbar}{i} \frac{\partial}{\partial q_{s(i)}}, \qquad i = 0, 1, \ldots, N-1. \tag{22}$$

The correspondence between the quantum-mechanical operator bracket and the classical Poisson bracket is straightforward (Rabei *et al.*, 2006):

$$\left[q_{r,s(i)}, p_{r,s(i)}\right]\Psi = \left[q_{r,s(i)} p_{r,s(i)} - p_{r,s(i)} q_{r,s(i)}\right]\Psi \tag{23}$$

$$\left[q_{r,s(i)}, p_{r,s(i)}\right] \Psi = \frac{\hbar}{i}\left[q_{s(i)}\frac{\partial}{\partial q_{s(i)}} - \frac{\partial}{\partial q_{s(i)}} q_{s(i)}\right] \Psi = i\hbar\Psi, \tag{24}$$

and the Schrödinger equation reads

$$H\Psi = i\hbar\frac{\partial}{\partial t}\Psi. \tag{25}$$

It follows that the commutators of the quantum-mechanical operators are proportional to the corresponding classical Poisson brackets (Rabei *et al.*, 2006):

$$\left[q_{r,s(i)}, p_{r,s(i)}\right] \leftrightarrow i\hbar \left\{q_{r,s(i)}, p_{r,s(i)}\right\}. \tag{26}$$

Further, we generalize Heisenberg's equation of motion for coordinate operators as follows (Rabei *et al.*, 2006):

$$\frac{d^{s(i+1)-s(i)}}{d(t-b)^{s(i+1)-s(i)}}\left\langle \hat{q}_{r,s(i)}\right\rangle = \frac{1}{i\hbar}\left\langle\left[\hat{q}_{r,s(i)}, \hat{H}\right]\right\rangle, \tag{27}$$

and for momentum operators:

$$(-1)^{s(i+1)-s(i)}\frac{d^{s(i+1)-s(i)}}{d(t-b)^{s(i+1)-s(i)}}\left\langle \hat{p}_{r,s(i)}\right\rangle = -\frac{1}{i\hbar}\left\langle\left[\hat{p}_{r,s(i)}, \hat{H}\right]\right\rangle. \tag{28}$$

Equations (27) and (28) are valid for integerorder derivatives as well as non-integer order.

4. QUANTIZING THE BROWNIAN MOTION

In reference to Eq. (1), the force acting on the Brownian particle is

$$F = -b\vec{v}(t) + \vec{R}(t). \tag{29}$$

To construct the Hamiltonian of the Brownian particle we should obtain the potential corresponding to this force. By using the formula (Rabei *et al.*, 2004)

$$U = (-1)^{-(\alpha+1)} \int \left[L^{-1}\left\{\frac{1}{S^{\alpha}} L\left(F(q_{\beta})\right)\right\}\right] dq_{\alpha}, \tag{30}$$

where $\beta = 2\alpha$; L and L^{-1} are the respective Laplace transform and inverse Laplace transform, one can derive the potential of a nonconservative force. The potential corresponding to the velocity-dependent term, which represents the dissipation effect, is

$$U = \frac{ib}{2} q_{1/2}^{2}. \tag{31}$$

The random force $\vec{R}(t)$ may be represented as a sequence of impulses, in much the same way as we think of pressure to be just the force per unit area arising from a tremendous number of impacts of individual molecules. Hence, we can replace the force of one impulse or one collision $R(t')$ by $a\delta(t'-t)$. Then $\vec{R}(t)$ could be written as the well-known formula (Duffy, 2001)

$$\vec{R}(t) = \int_0^{\infty} R(t')\,\delta(t'-t)\,dt. \tag{32}$$

The potential that corresponds to the one impulse or one collision $R(t')$ or $a\delta(t'-t)$ is

$$V(q_0) = -aq_0\,\delta(t'-t). \tag{33}$$

The Lagrangian of the Brownian particle is, therefore,

$$L = \frac{1}{2}mq_1^2 + \frac{ib}{2}q_{1/2}^2 + aq_0\delta(t'-t), \tag{34}$$

where

$$q_0 = x, \qquad q_1 = \frac{dx}{dt}, \qquad q_{1/2} = \frac{d^{1/2}x}{d(t-b)^{1/2}}, \tag{35}$$

and

$$s(0) = 0, \qquad s(1) = \frac{1}{2}, \qquad s(2) = 1. \tag{36}$$

The generalized Euler–Lagrange equation (Riewe, 1976, 1997) for this problem reads

$$\frac{\partial L}{\partial q_0} + (-1)^{1/2}\frac{d^{1/2}}{d(t-a)^{1/2}}\left(\frac{\partial L}{\partial q_{1/2}}\right) - \frac{d}{dt}\left(\frac{\partial L}{\partial q_1}\right) = 0. \tag{37}$$

This leads to

$$m\ddot{q} = -b\frac{d^{1/2}}{d(t-a)^{1/2}}q_{1/2} + a\,\delta(t'-t) = -b\dot{q} + R'(t), \tag{38}$$

which is the classical Langevin equation for one impulse or one collision; it is generalized to Eq. (1) for the overall random force.

The canonical momenta are (Riewe, 1976, 1997)

$$p_0 = \frac{\partial L}{\partial q_{1/2}} + i\frac{d^{1/2}}{d(t-a)^{1/2}}\frac{\partial L}{\partial q_1} = ibq_{1/2} + imq_{3/2}, \tag{39}$$

and

$$p_{1/2} = \frac{\partial L}{\partial q_1} = mq_1. \tag{40}$$

Making use of Eq. (16), we can write the Hamiltonian of the Brownian particles as

$$H = \frac{d^{1/2}}{d(t-b)^{1/2}}\,(q_0)\,p_0 + \frac{d^{1/2}}{d(t-b)^{1/2}}(q_{1/2})p_{1/2} - L = \frac{(p_{1/2})^2}{2m} + q_{_{1/2}}\,p_0 + \frac{b}{2i}q^2_{_{1/2}} - aq_0\,\delta(t'-t). \tag{41}$$

Here p_0 and $p_{1/2}$ are the canonical conjugate momenta to q_0 and $q_{1/2}$, respectively.

Using Eqs. (22), (25) and (41), we can write Schrödinger's equation as

$$i\hbar\frac{\partial}{\partial t}\Psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q_{1/2}^2} + \frac{\hbar}{i}q_{1/2}\frac{\partial}{\partial q_0} + \frac{1}{2i}bq_{1/2}^2 - aq_0\,\delta(t'-t)\right]\Psi. \tag{42}$$

Defining Ψ as

$$\Psi = F(q_{1/2}, q_0)T(t), \tag{43}$$

then, using the method of separation of variables, we obtain the following:

Assuming a constant q_0, and using the identity (Duffy, 2001)

$$f(t)\delta(t'-t) = f(t')\delta(t'-t), \tag{44}$$

we have for the time-dependent part:

$$i\hbar\frac{d}{dt}T + c\delta(t'-t) = E_0T, \tag{45}$$

which has the solution (Duffy, 2001)

$$T = \frac{T_0}{c}\exp\left[\frac{-i}{c\hbar}E_0(t'-t)\right]H(t'-t), \tag{46}$$

$H(t'-t)$ being the Heaviside step function; and for the other time-independent part:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2i}by^2 + \frac{\hbar}{i}y\frac{\partial}{\partial x}\right]F = E_0F, \tag{47}$$

where $q_0 = x$ and $q_{1/2} = y$. If we consider u as a constant, as an approximation, Eq. (47) will has the solution

$$F_n(y, x) = AH_n\left[\left(\frac{m\gamma}{i\hbar^2}\right)^{1/4} y\right]\exp\left[\frac{-(m\gamma/i\hbar^2)^{1/2}y^2}{2}\right]. \tag{48}$$

In terms of $q_{s(i)}$,

$$F_n\left(q_{1/2}, q_0\right) = AH_n\left[\left(\frac{m\gamma}{i\hbar^2}\right)^{1/4}\frac{q_0}{u}\right]\exp\left[\frac{-(m\gamma/i\hbar^2)^{1/2}q_0^2}{2u^2}\right], \tag{49}$$

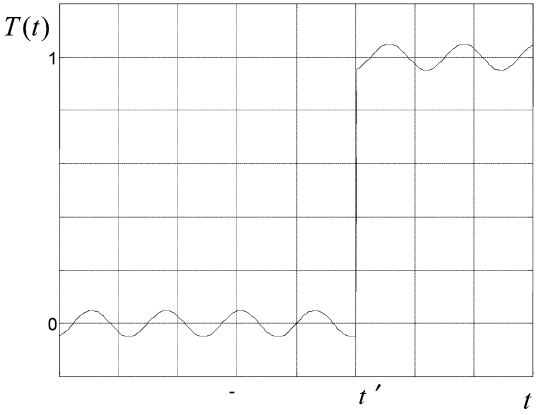

Fig. 1. : $T(t)$, the time-dependent part.

H_n being Hermite polynomials.

Thus,

$$\Psi_n = AH_n\left[\left(\frac{mb}{i\hbar^2}\right)^{1/4}\frac{q_0}{u}\right]\exp\left[\frac{-(mb/i\hbar^2)^{1/2}q_0^2}{2u}\right]$$
$$\times\exp\left[\frac{-i}{c\hbar}E_0(t'-t)\right]H(t'-t). \tag{50}$$

The canonical coordinates are q_0 and $q_{1/2}$. The wave function Ψ depends on these.

For a nondissipative and no-random-force system, $b = R(t) = 0$, Eq. (50) reduces to the wave function of the free particle with energy eigenvalue E.

The time-dependent part of Eq. (50) is represented schematically in Fig. 1. At $t = t'$ the δ-function effects appear clearly; while for $t \neq t'$ the ordinary time-dependent behavior of the free particle manifests itself.

5. CONCLUSION

The quantization of a system with Brownian motion has been carried out according to the theory we have proposed recently (Rabei *et al.*, 2006). A potential corresponding to the random force and a Hamiltonian are constructed. The relevant Schrödinger's equation has then been solved. The Langevin equation could be obtained easily from our Lagrangian. The plot represent random forces and hence the Brownian motion. The next step could be to study problems such as the correlation functions, diffusion process, transport equation, etc., on a quantum-mechanical basis.

APPENDIX

Fractional calculus

The fractional integral of a function *f*(*t*) is defined as (Oldham and Spanier, 1974; Carpintri and Mainardi, 1997)

$$J^{\alpha} f(t) \equiv \frac{1}{\Gamma(\alpha)} \int_a^t (t-\tau)^{\alpha-1} f(\tau)\, d\tau, \qquad \alpha \in \mathrm{R}^+, \tag{A.1}$$

where J^{α} represents the fractional integral operator of order a, and R^+ represents the set of positive real numbers.

If we introduce the positive integer m such that $m-1 < \alpha \leq m$, the fractional derivative of order $\alpha > 0$ may be defined as

$$D^{\alpha} f(t) = D^m J^{m-\alpha} f(t), \tag{A.2}$$

D^{α} being the fractional deferential operator of order α. Equation (2) may be rewritten using Eq. (1) as follows:

$$D^m f(t) \equiv \frac{d^m}{dt^m} \left[\frac{1}{\Gamma(m-\alpha)} \int_a^t \frac{f(\tau)}{(t-\tau)^{\alpha+1-m}} d\tau \right], \qquad m-1 < \alpha \leq m, \tag{A.3}$$

Here, we formulate the problem in terms of the left fractional derivative the left-Riemann–Liouville fractional derivatives, which are defined in Eqs. (A.1) and (A.2). Most of the left-fractional operations also hold for the right ones. For the left operations, in the interval $[a, b]$, $f(t)$ must vanish for $t < a$; while $f(t) = 0$ for $t > b$ for the right operation. Thus, the left operations are causal. Conversely, the right operations are anticausal (Dreisigmeyer and Young, 2003). From the physical point of view, when we differentiate with respect to time, the right differentiation represents an operation performed on the future state of the process $f(t)$ (Agrawal, 2002).

Fractional integral and differential operators have the following properties (Oldham and Spanier, 1974; Carpintri and Mainardi, 1997):

For I, the identity operator:

$$D^n J^n = I, \tag{A.4}$$

but the inverse application of the two operators is not necessarily true.

For $n > 0$, J^n and D^n are linear operators, i.e.,

$$J^n\, [f_1(x) + f_2(x)] = J^n f_1(x) + J^n f_2(x); \tag{A.5}$$

$$D^n\, [f_1(x) + f_2(x)] = D^n f_1(x) + D^n f_2(x). \tag{A.6}$$

For a constant c, J^n and D^n are homogeneous operators, i.e.,

$$J^n\, [cf(x)] = cJ^n f(x); \tag{A.7}$$

$$D^n\,[cf(x)] = cD^n f(x). \tag{A.8}$$

For $\alpha, \beta > 0$, J^n obeys the additive index law, but not necessarily D^n, i.e.,

$$J^\alpha J^\beta\,[f(x)] = J^{\alpha+\beta} f(x); \tag{A.9}$$

$$D^\alpha D^\beta\,[f(x)] \neq D^{\alpha+\beta} f(x). \tag{A.10}$$

Of special importance are the fractional integrals and fractional derivatives of the function $(t-a)^\beta$, which are given by

$$\frac{d^\alpha}{d(t-a)^\alpha}\,[t-a]^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha+1)}\,[t-a]^{\beta-\alpha}\,. \tag{A.11}$$

For $\alpha = 1/2$ this equation is called semi-derivative; for $\alpha = -1/2$ it is called semi-integral.

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