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Particle in a Finite Potential Well, with Dissipation

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Abstract: In this study fractional derivatives have been used to study a nonconservative system: free particle in a finite potential well, containing a dissipative medium. The Lagrangian and other classical functions have been introduced to take into account nonconservative effects. The canonical quantization of the system is carried out according to the Dirac method. A suitable Schrödinger equation is set up and solved for the Lagrangian representing this system.

Key words: Free particle in a bounded volume in space, hamiltonian formulation, canonical quantization, fractional calculus, nonconservative systems, dissipation

INTRODUCTION

Many attempts have been made to incorporate nonconservative forces into Lagrangian and Hamiltonian formulations; but those attempts could not give a completely consistent physical interpretation of these forces. The Rayleigh dissipation function, invoked when the frictional force is proportional to the velocity (Goldstein, 1980), was the first to be used to describe frictional forces in the Lagrangian. However, in that case, another scalar function was needed, in addition to the Lagrangian, to specify the equations of motion. At the same time, this function does not appear in the Hamiltonian. Accordingly, the whole process is of no use when it is attempted to quantize nonconservative systems.

The most substantive work in this context was that of Riewe (1996 and 1997), who used fractional derivatives to study nonconservative systems and was able to generalize the Lagrangian and other classical functions to take into account nonconservative effects. Rabei *et al.* (2004) developed a general formula for the potential of any arbitrary force, conservative or nonconservative. This led directly to the consideration of the dissipative effects in Lagrangian and Hamiltonian formulations.

In this study we wish to apply the method of quantizing nonconservative, or dissipative, systems using fractional calculus (Rabei *et al.* 2006 a, b) to a system of free particle in a bounded volume in space, a finite potential well, containing a dissipative medium.

QUANTIZATION OF NONCONSERVATIVE SYSTEMS

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

This canonical conjugate relation was obtained directly from Hamilton's equation defined by Riewe (1996 and 1997) as follows:

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

Rabie *et al.* (2006a and b) concluded that $p_{r,s(i)}$ is the canonical conjugate of $q_{r,s(i)}$. Accordingly, the Hamiltonian can be written in the following form:

$$\begin{aligned} H &= \sum_{i=0}^{N-1} \frac{d^{s(i+1)-s(i)}}{d(t-a)^{s(i+1)-s(i)}} q_{r,s(i)} p_{r,s(i)} - L, \quad 0 \le i \le N-1 \\ &= \sum_{i=0}^{N-1} q_{r,s(i+1)} p_{r,s(i)} - L \end{aligned} \tag{2}$$

The last result, Eq. 2, is equivalent to Riewe's Hamiltonian (Riewe, 1996, 1997) and it is applicable to higher-order Lagrangian with integer derivatives, as obtained by Pimental and Teixeira (1997).

The most general classical Poisson bracket for any two functions was defined, F and G, in phase space (Rabei *et al.*, 2006a, b) as follows:

$$\{F,G\} = \sum_{k=0}^{N-1} \frac{\partial F}{\partial q_{r,s(k)}} \frac{\partial G}{\partial p_{r,s(k)}} - \frac{\partial F}{\partial p_{r,s(k)}} \frac{\partial G}{\partial q_{r,s(k)}} \tag{3}$$

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

$$\left\{q_{r,s(i)},p_{l,s(j)}\right\}=\sum_{k=0}^{N-1}\frac{\partial q_{r,s(i)}}{\partial q_{m,s(k)}}\frac{\partial p_{l,s(j)}}{\partial p_{m,s(k)}}-\frac{\partial q_{r,s(i)}}{\partial p_{m,s(k)}}\frac{\partial p_{l,s(j)}}{\partial q_{m,s(k)}},\quad 0\le i,j\le N-1 \tag{4}$$

$$=\delta_{ij}\delta_{rl} \tag{5}$$

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

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

$$\frac{d^{s(i+1)-s(i)}}{d(t-a)^{s(i+1)-s(i)}}q_{r,s(i)}=q_{r,s(i+1)}=\left\{q_{r,s(i)},H\right\} \tag{6}$$

and

$$\left(-1\right)^{s(i+1)-s(i)}\frac{d^{s(i+1)-s(i)}}{d(t-a)^{s(i+1)-s(i)}}p_{r,s(i)}=-\left\{p_{r,s(i)},H\right\} \tag{7}$$

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

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

$$p_{s(i)}\quad\frac{\hbar}{i}\frac{\partial}{\partial q_{s(i)}},\qquad i=0,1,...,N-1. \tag{8}$$

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

$$\left[q_{r,s(i)},p_{r,s(i)}\right]\Psi=\left[q_{r,s(i)}p_{r,s(i)}-p_{r,s(i)}q_{r,s(i)}\right]\Psi=i\hbar\Psi \tag{9}$$

and the Schrödinger equation reads

$$H\Psi=i\hbar\frac{\partial}{\partial t}\Psi \tag{10}$$

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

$$q_{r,s(i)},p_{r,s(i)}\qquad i\hbar\left\{q_{r,s(i)},p_{r,s(i)}\right\} \tag{11}$$

Further, Rabie *et al.* (2006a and b) generalize Heisenberg's equation of motion for coordinate operators as follows:

$$\frac{d^{s(i+1)-s(i)}}{d(t-a)^{s(i+1)-s(i)}}\left\langle\hat{q}_{r,s(i)}\right\rangle=\frac{1}{i\hbar}\ \hat{q}_{r,s(i)},\hat{H} \tag{12}$$

and for momentum operators:

$$(-1)^{s(i+1)-s(i)}\frac{d^{s(i+1)-s(i)}}{d(t-a)^{s(i+1)-s(i)}}\hat{p}_{r,s(i)}=-\frac{1}{i\hbar}\ \hat{p}_{r,s(i)},\hat{H} \tag{13}$$

Equation 12 and 13 are valid for integer-order derivatives as well as non-integer order.

Finite square potential well containing dissipative medium: Suppose a one dimensional finite square well of width 2a and a potential (Griffiths, 1995; Merzbacher, 1970).

$$V(x)=\begin{matrix}-V_0, & \text{if } -a<x<a\\ 0, & \text{otherwise}\end{matrix} \tag{14}$$

where V_0 is a (positive) constant. The finite square well admits both bound states (with E<0) and scattering states (with E>0). In the regions x<-a and x>a the potential is zero, so the Schrödinger Eq. reads:

$$E\Psi=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi\ \text{ or }\ k^2\Psi=\frac{\partial^2}{\partial x^2}\Psi \tag{15}$$

with a physically admissible solution is

$$\Psi(x)=\begin{cases}A\exp kx\text{ , for } x<-a\\ B\exp-kx\text{ , for } x>a\end{cases} \tag{16}$$

In the region -a<x<a the potential is $-V_0$, so the Schrödinger Eq. reads:

$$E\Psi=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi-V_0\Psi\ \text{ or }\ -\ell\Psi=\frac{\partial^2}{\partial x^2}\Psi \tag{17}$$

with a general solution is

$$\Psi(x)=D\cos(\ell x)\text{ , for -a}<x<a \tag{18}$$

In the following we are going to treat the same problem with a viscous material filling the whole space.

Consider a particle moving in the dissipative medium, the viscous force on the particle vary as the first power of its speed, i.e.,

$$F = -\gamma q_1 \quad (19)$$

γ being a positive constant. Using the formula given by Rabei *et al.* (2004)

$$U = (-1)^{-(\alpha+1)} \int \left[L^{-1} \left\{ \frac{1}{S^{\alpha}} L\left(F(q_{\beta})\right) \right\} \right] dq_{\alpha} \quad (20)$$

one can derive the potential of a nonconservative force. The potential corresponding to this dissipation is

$$U = \frac{i\gamma}{2} q_{1/2}^2 \quad (21)$$

In the regions x<-a and x>a the Lagrangian is:

$$L = \frac{1}{2} m q_1^2 - \frac{i\gamma}{2} q_{1/2}^2 \quad (22)$$

where

$$q_0 = x, \quad q_1 = \frac{dx}{dt}, \quad q_{1/2} = \frac{d^{1/2} x}{d(t-a)^{1/2}} \quad (23)$$

and

$$s(0) = 0, s(1) = 1/2, \ s(2) = 1 \quad (24)$$

The generalized Euler-Lagrange equation for this problem reads

$$\frac{\partial L}{\partial q_0} + (-1)^{1/2} \frac{d^{1/2}}{d(t-a)^{1/2}} \frac{\partial L}{\partial q_{1/2})} - \frac{d}{dt}\frac{\partial L}{\partial q_1} = 0 \quad (25)$$

Substituting the Lagrangian given by Eq. 22, we obtain the equation of motion

$$m\ddot{q} + \gamma\dot{q} = 0 \quad (26)$$

The canonical momenta are

$$p_0 = \frac{\partial L}{\partial q_{1/2}} + i \frac{d^{1/2}}{d(t-a)^{1/2}} \frac{\partial L}{\partial q_1} = i\gamma\, q_{1/2} + im q_{3/2} \quad (27)$$

and

$$p_{1/2} = \frac{\partial L}{\partial q_1} = m q_1 \quad (28)$$

Making use of Eq. 2, we have for the Hamiltonian

$$H = \frac{d^{1/2}}{d(t-a)^{1/2}}(q_0)p_0 + \frac{d^{1/2}}{d(t-a)^{1/2}}\left(q_{1/2}\right)p_{1/2} - L$$
$$= \frac{\left(p_{1/2}\right)^2}{2m} + q_{1/2} p_0 + \frac{\gamma}{2i} q_{1/2}^2 \quad (29)$$

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

With Eq. 8, 10 and 29, Schrödinger's equation reads

$$i\hbar \frac{\partial}{\partial t}\Psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q_{1/2}^1} + \frac{\hbar}{i} q_{1/2} \frac{\partial}{\partial q_0} + \frac{1}{2i}\gamma q_{1/2}^2 \right]\Psi \quad (30)$$

This is Schrödinger's equation for a free particle in a finite potential well containing a dissipative medium. Using the method of separation of variables, we obtain the following:

the time-dependent part:

$$T = T_0 \exp\frac{-iE_0 t}{\hbar} \quad (31)$$

and the other, time-independent, part:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2i}\gamma y^2 + \frac{\hbar}{i} y \frac{\partial}{\partial x} \right] F = E_0 F \quad (32)$$

where $q_0 = x$ and $q_{1/2} = y$. Letting $x = uy$ and substituting into Eq. 32, we have:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2i}\gamma y^2 + \frac{\hbar}{i}\frac{\partial}{\partial u} \right] F = E_0 F \quad (33)$$

The y-part reads

$$\left[\frac{d^2}{dy^2} - \left(\frac{m\gamma}{i\hbar^2}\right) y^2 \right] Y = -2E_y \left(\frac{m}{\hbar^2}\right) Y \quad (34)$$

This has the solution (Dass and Sharma, 1998; Arfken, 1985):

$$Y_n = Y_0 H_n\left[\left(\frac{m\gamma}{i\hbar^2}\right)^{\frac{1}{4}} y\right]\exp\frac{-\left(\frac{m\gamma}{i\hbar^2}\right)^{\frac{1}{2}} y^2}{2} \tag{35}$$

where H_n are Hermite polynomials.
The u-part of Eq. 53 reads

$$\frac{\hbar}{i}\frac{d}{du} - E_x\ U = 0 \tag{36}$$

which has the solution:

$$U = U_0 \cos\frac{E_x u}{\hbar} \tag{37}$$

by considering the boundary conditions $\Psi = 0$.

The energy eigenvalues

$$E_{y.n} = \frac{1}{2}(2n+1)\hbar\left(\frac{i\gamma}{m}\right) \text{ and } E_{x.n} = \frac{n\pi\hbar}{2a} \tag{38}$$

Thus,

$$\Psi_n = AH_n\left[\left(\frac{m\gamma}{i\hbar^2}\right)^{\frac{1}{4}} q_{\frac{1}{2}}\right]\exp\frac{-\left(\frac{m\gamma}{i\hbar^2}\right)^{\frac{1}{2}} q^2_{\frac{1}{2}}}{2} \cos\left(\frac{E_{q_0}}{\hbar q_{\frac{1}{2}}}\right)q_0 \exp\left(\frac{-i}{\hbar}E_0 t\right) \tag{39}$$

The wave function Ψ depends on canonical coordinates q_0 and $q_{1/2}$. The total energy eigenvalues:

$$E_n = E_{y.n} + E_{x.n} = \frac{1}{2}(2n+1)\hbar\left(\frac{i\gamma}{m}\right) + \frac{n\pi\hbar}{2a},\ n = 1, 2,.. \tag{40}$$

the drag force effects are represented clearly in the wave function and in the energy eigenvalues.

In the region $-a<x<a$ the potential is $-V_0$, the Lagrangian is

$$L = \frac{1}{2}mq_1^2 - \frac{i\gamma}{2}q^2_{\frac{1}{2}} + V \tag{41}$$

Making use of Eq. 3, we have for the Hamiltonian

$$H = \frac{(p_{\frac{1}{2}})^2}{2m} + q_{\frac{1}{2}}p_0 + \frac{\gamma}{2i}q^2_{\frac{1}{2}} - V \tag{42}$$

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

With Eq. 8, 10 and 29, Schrödinger's Eq. reads:

$$i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2_{1/2}} + \frac{\hbar}{i}q_{1/2}\frac{\partial}{\partial q_0} + \frac{1}{2i}\gamma q^2_{1/2} - V\right]\Psi \tag{43}$$

with the solution

$$\psi_n = AH_n\left[\left(\frac{m\gamma}{i\hbar^2}\right)^{\frac{1}{4}} q_{\frac{1}{2}}\right]\exp\frac{-\left(\frac{m\gamma}{i\hbar^2}\right)^{\frac{1}{2}} q^2_{\frac{1}{2}}}{2} \cos\left(\frac{E_{q_0}}{\hbar q_{\frac{1}{2}}}\right)q_0 \exp\left[\frac{-i}{\hbar}(E_0 - V)t\right] \tag{44}$$

CONCLUSION

The quantization of nonconservative system: a particle in a finite potential well containing dissipative medium has been carried out according to the theory, which has proposed recently. A potential corresponding to the viscous force and a Hamiltonian are constructed. The relevant Schrödinger's equation has then been set up and solved. The viscous forces effects and hence the dissipation are represented clearly in the resultant wave function.

APPENDIX

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

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

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

If we introduce the positive integer m such that $-1<\alpha\leq m$, 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 A-2 may be rewritten using Eq. A-1 as follows:

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

Here, we formulate the problem in terms of the left fractional derivative the left Riemann-Liouville fractional derivatives, which are defined in Eq. (A-1, A-2). Most of the left fractional operations also hold for the right ones. For the left operations 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 anti-causal (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, 2001).

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

$$D^n J^n = I \qquad \text{(A-4)}$$

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.

$$J^n\left[f_1(x)+f_2(x)\right] = J^n f_1(x) + J^n f_2(x) \qquad \text{(A-5)}$$

$$D^n\left[f_1(x)+f_2(x)\right] = D^n f_1(x) + D^n f_2(x) \qquad \text{(A-6)}$$

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

$$J^n\left[cf(x)\right] = cJ^n f(x) \qquad \text{(A-7)}$$

$$D^n\left[cf(x)\right] = cD^n f(x) \qquad \text{(A-8)}$$

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

$$J^\alpha J^\beta\left[f(x)\right] = J^{\alpha+\beta} f(x) \qquad \text{(A-9)}$$

$$D^\alpha D^\beta\left[f(x)\right] \neq D^{\alpha+\beta} f(x) \qquad \text{(A-10)}$$

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

$$\frac{d^\alpha}{d(t-a)^\alpha}\left[t-a\right]^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha+1)}\left[t-a\right]^{\beta-\alpha} \qquad \text{(A-11)}$$

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

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