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EXACT SOLUTIONS TO FICK-JACOBS EQUATION

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Abstract: A relation between Fick-Jacobs and Schrödinger equation is shown. When the diffusion coefficient is constant, exact solutions for Fick-Jacobs equation are obtained. Using a change of variable the general case is studied.

1. Introduction

Recently, methods of quantum physics haven been used to solve problems in other disciplines. For instance, Black-Scholes can be mapped to Schrödinger equation [1, 2, 3]. It is worth to mention that Black-Scholes equation plays an important role in finance [1, 2, 3]. Moreover, it is well known that the Fick equation represents the simplest model of diffussion. The Fick equation can be mapped to Schrödinger equation too. When the diffusion is in a channel which has shape of surface of revolution with cross section of area $A(x)$, the Fick equation is changed to Fick-Jacobs equation [4]

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x)A(x)\frac{\partial}{\partial x}\left(\frac{C(x,t)}{A(x)}\right)\right], \qquad (1.1)$$

where $C(x,t)$ is the concentration of particles and $D(x)$ is the diffusion coefficient.

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The Fick-Jacobs equation is important to study diffusion in biological channels or zeolites and is studied with perturbative and numerical methods [5, 6, 7, 8, 9, 10, 11]. In this paper we find a relation between Fick-Jacobs and Schrödinger equation. Also, using quantum mechanics methods, we obtain exact solutions for Fick-Jacobs equation, in particular when the diffusion coefficient is constant and the shape of channel is conical, throat-like, sinusoidal or Gaussian. To study the Fick-Jacobs equation with constant diffusion coefficient, we use the operator

$$\hat{P}_{(f)} = -i\frac{\partial}{\partial x} + i\frac{\partial f(x)}{\partial x}, \qquad x \in \mathbb{R} \tag{1.2}$$

where f is smooth function. The operator (1.2) was first studied by P. A. M. Dirac [12]. The general case is studied with a change of variable.

This paper is organized as follows: In Section 2 a review of quantum mechanics with a generalized operator (1.2) is presented. In Section 3 is shown a relation between Fick-Jacobs and Schrödinger equation. In Section 4 some properties of solutions are considered. In Section 5 the case with constant diffusion coefficient is studied for different examples. In Section 6 the general case is analyzed. Finally in Section 7 a summary is given.

2. Generalized Momentum Operator

The Hermitian operator

$$\hat{P} = -i\frac{\partial}{\partial x} \tag{2.1}$$

is the usual momentum operator in quantum mechanics, with $\hbar = 1$. However, in early quantum mechanics, P. A. M. Dirac studied the no-Hermitean operator [12]

$$\hat{P}_{(f)} = e^{f(x)}\hat{P}e^{-f(x)} = \hat{P} + i\frac{\partial f(x)}{\partial x}. \tag{2.2}$$

This operator is very interesting, for example using it we can build a supersymmetric quantum mechanics. In fact, lets us propose the Hermitian Hamiltonians:

$$\hat{H}_1 = \alpha^2 \hat{P}_{(f)}^\dagger \hat{P}_{(f)} = \alpha^2 \left(\hat{P}^2 + \frac{d^2 f}{dx^2} + \left(\frac{df}{dx}\right)^2 \right), \tag{2.3}$$

$$\hat{H}_2 = \alpha^2 \hat{P}_{(f)} \hat{P}^\dagger_{(f)} = \alpha^2 \left(\hat{P}^{\,2} - \frac{d^2 f}{dx^2} + \left(\frac{df}{dx} \right)^2 \right), \qquad (2.4)$$

here α is constant. Now, if W is a smooth function, we can propose

$$f(x) = \int_0^x W(u) du, \qquad x \geq 0, \qquad (2.5)$$

then

$$\hat{H}_1 = \alpha^2 \left(\hat{P}^{\,2} + \frac{dW}{dx} + W^2 \right), \qquad (2.6)$$

$$\hat{H}_2 = \alpha^2 \left(\hat{P}^{\,2} - \frac{dW}{dx} + W^2 \right). \qquad (2.7)$$

These Hamiltonians can be used to form the matrix

$$\hat{\mathcal{H}} = \begin{pmatrix} \hat{H}_1 & 0 \\ 0 & \hat{H}_2 \end{pmatrix}. \qquad (2.8)$$

According to the supersymmetric quantum mechanics [13], $\hat{\mathcal{H}}$ represents a superhamiltonian.

Furthermore, with the operator (2.2) we can build the Hamiltonians:

$$\hat{H}_3 = \beta^2 \hat{P}^\dagger_{(f)} \hat{P}^\dagger_{(f)} = \beta^2 \left(\hat{P}^2 - 2i \frac{df}{dx} \hat{P} - \frac{d^2 f}{dx^2} - \left(\frac{df}{dx} \right)^2 \right), \qquad (2.9)$$

$$\hat{H}_4 = \beta^2 \hat{P}_{(f)} \hat{P}_{(f)} = \beta^2 \left(\hat{P}^2 + 2i \frac{df}{dx} \hat{P} + \frac{d^2 f}{dx^2} - \left(\frac{df}{dx} \right)^2 \right), \qquad (2.10)$$

where β is constant. These Hamiltonians are no-Hermitian, however with them we can construct Hamiltonians which arise in the so-called quantum finance [3]. We will use these Hamiltonians to study Fick-Jacobs equation.

Now, using the Hamiltonians $\hat{H}_3$ and $\hat{H}_4$, we can set the wave equations

$$i \frac{\partial \psi_3(x,t)}{\partial t} = \hat{H}_3 \psi_3(x,t), \qquad (2.11)$$

$$i \frac{\partial \psi_4(x,t)}{\partial t} = \hat{H}_4 \psi_4(x,t). \qquad (2.12)$$

Both of these equtions are equivalent to non-relativistic free particle. In fact, first note that

$$\hat{P}^\dagger_{(f)} \hat{P}^\dagger_{(f)} = e^{-f(x)} \hat{P} e^{f(x)} e^{-f(x)} \hat{P} e^{f(x)} = e^{-f(x)} \hat{P}^2 e^{f(x)},$$

$$\hat{P}_{(f)}\hat{P}_{(f)} = e^{f(x)}\hat{P}e^{-f(x)}e^{f(x)}\hat{P}e^{-f(x)} = e^{f(x)}\hat{P}^2e^{-f(x)}, \qquad (2.13)$$

namely

$$i\frac{\partial\psi_3(x,t)}{\partial t} = \hat{H}_3\psi_3(x,t) = \beta^2 e^{-f(x)}\hat{P}^2 e^{f(x)}\psi_3(x,t),$$

$$i\frac{\partial\psi_4(x,t)}{\partial t} = \hat{H}_4\psi_4(x,t) = \beta^2 e^{f(x)}\hat{P}^2 e^{-f(x)}\psi_4(x,t),$$

thus

$$i\frac{\partial\left(e^{f(x)}\psi_3(x,t)\right)}{\partial t} = \beta^2\hat{P}^2\left(e^{f(x)}\psi_3(x,t)\right),$$

$$i\frac{\partial\left(e^{-f(x)}\psi_4(x,t)\right)}{\partial t} = \beta^2\hat{P}^2\left(e^{-f(x)}\psi_4(x,t)\right).$$

These equations represent the free particle wave equation and their solutions are:

$$e^{f(x)}\psi_3(x,t) = e^{-i\beta^2\hat{P}^2 t}\left(e^{f(x)}\psi_{03}(x)\right),$$

$$e^{-f(x)}\psi_4(x,t) = e^{-i\beta^2\hat{P}^2 t}\left(e^{-f(x)}\psi_{04}(x)\right), \qquad (2.14)$$

where $\psi_3(x,0) = \psi_{03}(x)$ and $\psi_4(x,0) = \psi_{04}(x)$ are the initial conditions. Therefore,

$$\psi_3(x,t) = \left(e^{-f(x)}e^{-i\beta^2\hat{P}^2 t}e^{f(x)}\right)\psi_{03}(x),$$

$$\psi_4(x,t) = \left(e^{f(x)}e^{-i\beta^2\hat{P}^2 t}e^{-f(x)}\right)\psi_{04}(x) \qquad (2.15)$$

are the general solution of equations (2.11) and (2.12).

Also, if V is a potential, we can prove that the wave equations

$$i\frac{\partial\psi_3(x,t)}{\partial t} = \left(\beta^2\hat{P}^\dagger_{(f)}\hat{P}^\dagger_{(f)} + V(x)\right)\psi_3(x,t) \qquad (2.16)$$

$$i\frac{\partial\psi_4(x,t)}{\partial t} = \left(\beta^2\hat{P}_{(f)}\hat{P}_{(f)} + V(x)\right)\psi_4(x,t), \qquad (2.17)$$

are equivalent to

$$i\frac{\partial\left(e^{f(x)}\psi_3(x,t)\right)}{\partial t} = \hat{H}\left(e^{f(x)}\psi_3(x,t)\right), \qquad (2.18)$$

$$i\frac{\partial\left(e^{-f(x)}\psi_4(x,t)\right)}{\partial t} = \hat{H}\left(e^{-f(x)}\psi_4(x,t)\right), \qquad (2.19)$$

here the Hamiltonian is

$$\hat{H} = \beta^2 \hat{P}^2 + V(x). \tag{2.20}$$

The general solutions of the equations (2.18) and (2.19) are:

$$e^{f(x)}\psi_3(x,t) = e^{-i\hat{H}t}\left(e^{f(x)}\psi_{03}(x)\right), \tag{2.21}$$

$$e^{-f(x)}\psi_4(x,t) = e^{-i\hat{H}t}\left(e^{-f(x)}\psi_{04}(x)\right), \tag{2.22}$$

therefore, the general solutions of the equations (2.16) and (2.17) are given by

$$\psi_3(x,t) = \left(e^{-f(x)}e^{-i\hat{H}t}e^{f(x)}\right)\psi_{03}(x), \tag{2.23}$$

$$\psi_4(x,t) = \left(e^{f(x)}e^{-i\hat{H}t}e^{-f(x)}\right)\psi_{04}(x), \tag{2.24}$$

where the initial conditions are $\psi_3(x,0) = \psi_{03}(x)$ and $\psi_4(x,0) = \psi_{04}(x)$.

In the next section we will use these results to show a equivalence between Fick-Jacobs and Schrödinger equation.

3. Fick-Jacobs Equation as Schrödinger Equation

The Fick-Jacobs equation (1.1) can be written as

$$\frac{\partial C(x,t)}{\partial t} = D(x)\frac{\partial^2 C(x,t)}{\partial x^2} + D(x)\frac{\partial}{\partial x}\left[\ln\left(\frac{D(x)}{A(x)}\right)\right]\frac{\partial C(x,t)}{\partial x}$$
$$- \frac{\partial}{\partial x}\left(D(x)\frac{\partial \ln A(x)}{\partial x}\right)C(x,t). \tag{3.1}$$

Now, with the change of variable

$$y = \int_{x_0}^{x} \frac{dz}{\sqrt{D(z)}}, \qquad x_0 = \text{constant}, \tag{3.2}$$

we have

$$\frac{\partial}{\partial x} = \frac{1}{\sqrt{D(x)}}\frac{\partial}{\partial y}, \quad D(x)\frac{\partial^2}{\partial x^2} = \frac{\partial^2}{\partial y^2} - \frac{\partial\left(\sqrt{D(x)}\right)}{\partial x}\frac{\partial}{\partial y}. \tag{3.3}$$

Using (3.3) in (3.1), we get

$$\frac{\partial C(y,t)}{\partial t} = \frac{\partial^2 C(y,t)}{\partial y^2} + \sqrt{D(x)}\frac{\partial}{\partial x}\left(\ln\left[\frac{\sqrt{D(x)}}{A(x)}\right]\right)\frac{\partial C(y,t)}{\partial y}$$

$$-\frac{\partial}{\partial x}\left(D(x)\frac{\partial \ln A(x)}{\partial x}\right)C(y,t). \tag{3.4}$$

Whether the change of variable (3.2) is invertible, this equation can be written as a function of variable y. Also, if (3.2) is invertible, we can define the functions:

$$\frac{\partial}{\partial y}f(y) = -\frac{1}{2}\sqrt{D(x)}\frac{\partial}{\partial x}\left[\ln\left(\frac{\sqrt{D(x)}}{A(x)}\right)\right],$$

$$V(y) = \left(\frac{\partial f(y)}{\partial y}\right)^2 - \frac{\partial^2 f(y)}{\partial y^2} + \frac{\partial}{\partial x}\left(D(x)\frac{\partial \ln A(x)}{\partial x}\right). \tag{3.5}$$

Then (3.4) can be written as

$$-\frac{\partial C(y,t)}{\partial t} = \hat{H}_f C(y,t), \tag{3.6}$$

here

$$\hat{H}_f = \hat{P}^2 + 2i\frac{\partial f(y)}{\partial y}\hat{P} + \frac{\partial^2 f(y)}{\partial y^2} - \left(\frac{\partial f(y)}{\partial y}\right)^2 + V(y), \quad \hat{P} = -i\frac{\partial}{\partial y}.$$

Moreover, using the results of Section 2, we obtain

$$\hat{H}_f = e^{f(y)}\hat{H}e^{-f(y)}, \qquad \hat{H} = \hat{P}^2 + V(y), \tag{3.7}$$

then

$$-\frac{\partial C(y,t)}{\partial t} = e^{f(y)}\hat{H}e^{-f(y)}C(y,t), \tag{3.8}$$

namely

$$-\frac{\partial\left(e^{-f(y)}C(y,t)\right)}{\partial t} = \hat{H}\left(e^{-f(y)}C(y,t)\right) \tag{3.9}$$

and the solution of this equation is given by

$$e^{-f(y)}C(y,t) = e^{-\hat{H}t}\left(e^{-f(y)}C_0(y)\right). \tag{3.10}$$

Thus, when the change of variables (3.2) is invertible, the general solution of Fick-Jacobs equation is

$$C(y,t) = \left(e^{f(y)}e^{-\hat{H}t}e^{-f(y)}\right)C_0(y), \tag{3.11}$$

with the initial condition $C(y,0) = C_0(y)$.

There are several examples where the change of variable (3.2) is invertible, for instance $D = \text{constant}$, $D(x) = x^n, n = 1, 2, \cdots$, or $D(x) = e^{\alpha x}$, $\alpha \in \mathbb{R}$.

4. Some Properties of Solutions

Now we will study some solutions properties of Fick-Jacobs equation.

First, lets us take

$$C_0(y) = e^{f(y)}, \tag{4.1}$$

then the solution (3.11) gives

$$C(y,t) = e^{f(y)}. \tag{4.2}$$

Namely, in this case the system does not evolve. It is a interesting result, because in this case there is not diffusion.

Now, whether we want to find the evolution of any condition initial, we can use quantum mechanics results. For example, when the Hamiltonian is

$$\hat{H} = \hat{P}^2, \tag{4.3}$$

and initial condition is

$$C_0(y) = e^{f(y)} \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-\frac{(y-a_0)^2}{4\sigma^2}}, \qquad a_0, \sigma = \text{constant}, \tag{4.4}$$

using quantum mechanics results, we get

$$C(y,t) = e^{f(y)} \left(\frac{\sigma^2}{2\pi}\right)^{1/4} \frac{1}{(\sigma^2+t)^{1/2}} e^{-\frac{(y-a_0)^2}{4(\sigma^2+t)}}. \tag{4.5}$$

In general, if $\hat{H}\psi_n(y) = E_n\psi_n(y)$ and the concentration initial is

$$C_0(y) = e^{f(y)}\phi_0(y). \tag{4.6}$$

with

$$\phi_0(y) = \sum_{n\geq 0} a_n\psi_n(y), \tag{4.7}$$

where a_n are Fourier coefficients, then

$$C(y,t) = \sum_{n\geq 0} a_n e^{f(y)} e^{-E_n t}\psi_n(x).$$

Thus, as the Fick equation, the solution of Fick-Jacobs equation can be seen as quantum states.

5. Fick-Jacobs Equation with Constant Diffusion Coefficient

In this section we study the particular case $D = D_0 = \text{constant}$.

For this case the general solution is given by

$$C(x,t) = \sqrt{A(x)}e^{-\hat{H}t}\left(\frac{C_0(x)}{\sqrt{A(x)}}\right), \tag{5.1}$$

with

$$\hat{H} = D_0\left(\hat{P}^2 + V(x)\right), \qquad \hat{P} = -i\frac{\partial}{\partial x}, \tag{5.2}$$

$$V(x) = \frac{1}{2}\frac{1}{A(x)}\frac{\partial^2 A(x)}{\partial x^2} - \frac{1}{4}\left(\frac{\partial \ln A(x)}{\partial x}\right)^2. \tag{5.3}$$

Now lets us consider the following geometries:

5.1. Canonical Channel

When the channel is a cone, the cross-sectional area is $A(x) = \pi(1+\lambda x)^2$, where λ is the slope of the generatriz of the cone. For this case, the potential (5.3) is

$$V(x) = 0. \tag{5.4}$$

Then, using the results of Section 3, we find

$$C(x,t) = (1 + \lambda x)e^{-D_0\hat{P}^2}\left(\frac{C_0(x)}{1 + \lambda x}\right), \tag{5.5}$$

here the initial condition $C(x,0) = C_0(x)$ is satisfied.

In particular case

$$C_0(x) = \frac{(1 + \lambda x)}{(2\pi\sigma^2)^{1/2}}e^{-\frac{(x-a_0)^2}{4\sigma^2}}, \tag{5.6}$$

we get

$$C(x,t) = (1 + \lambda x)\left(\frac{\sigma^2}{2\pi}\right)^{1/4}\frac{1}{(\sigma^2 + tD_0)^{1/2}}e^{-\frac{(x-a_0)^2}{4(\sigma^2+tD_0)}}. \tag{5.7}$$

The conical tube was solved in [8] with a particular initial condition, here we solve the equation in general.

5.2. Throat-Like Channel

If the channel is a throat-like, the cross-sectional area can be taken as an exponential function

$$A(x) = e^{\alpha x + \beta}, \tag{5.8}$$

where α and β are constants. In this case the potential (5.3) is

$$V(x) = \frac{\alpha^2}{4}. \tag{5.9}$$

Therefore, the general solution is

$$C(x,t) = e^{-\frac{D_0 \alpha^2 t}{4}} e^{\frac{\alpha x}{2}} e^{-D_0 \hat{P}^2 t} e^{-\frac{\alpha x}{2}} C_0(x). \tag{5.10}$$

Then, when the initial condition is a Gaussian

$$C_0(x) = \frac{e^{\frac{\alpha}{2} x}}{(2\pi\sigma^2)^{1/2}} e^{-\frac{(x-a_0)^2}{4\sigma^2}}, \tag{5.11}$$

the concentration for any time is

$$C(x,t) = e^{-\frac{D_0 \alpha^2 t}{4}} e^{\frac{\alpha x}{2}} \left(\frac{\sigma^2}{2\pi}\right)^{1/4} \frac{1}{(\sigma^2 + tD_0)^{1/2}} e^{-\frac{(x-a_0)^2}{4(\sigma^2 + tD_0)}}. \tag{5.12}$$

5.3. Sinusoidal Channel

If the channel is sinusoidal, the cross section is

$$A(x) = B \left(\sin \gamma x\right)^2, \qquad B, \gamma = \text{constants.} \tag{5.13}$$

In this case the potential (5.3) is

$$V(x) = -\gamma^2. \tag{5.14}$$

Then the solution is

$$C(x,t) = e^{D_0 \gamma^2 t} \sin(\gamma x) e^{-D_0 \hat{P}^2 t} \frac{C_0(x)}{\sin(\gamma x)}. \tag{5.15}$$

When condition initial a Gaussian

$$C_0(x) = \frac{\sin(\gamma x)}{(2\pi\sigma^2)^{1/2}} e^{-\frac{(x-a_0)^2}{4\sigma^2}}, \tag{5.16}$$

the concentration for any time is

$$C(x,t) = e^{D_0 \gamma^2 t} \sin(\gamma x) \left(\frac{\sigma^2}{2\pi}\right)^{1/4} \frac{1}{(\sigma^2 + tD_0)^{1/2}} e^{-\frac{(x-a_0)^2}{4(\sigma^2 + tD_0)}}. \tag{5.17}$$

5.4. Gaussian Channel

Whether the area of the cross section of the channel is a Gaussian, we have

$$A(x) = e^{ax^2+bx+c}, \tag{5.18}$$

here a, b and c are constants. In this case the potential defined in (5.3) is

$$V(\zeta) = a^2\zeta^2 + a, \quad \text{with} \quad \zeta = x + \frac{b}{a}, \tag{5.19}$$

and the general solution is

$$C(\zeta,t) = e^{-D_0 at} e^{\frac{a\zeta^2}{2}} e^{-\hat{h}t} e^{-\frac{a\zeta^2}{2}} C_0(\zeta), \tag{5.20}$$

where

$$\hat{h} = D_0 \left(\hat{P}^2 + a^2\zeta^2 \right), \tag{5.21}$$

When we define $m = 1/(2D_0)$ and $\omega^2 = 4D_0^2 a^2$, the operator (5.21) is the Hamiltonian oscillator harmonic. Then, if $\psi_n(\zeta)$ is eigenfunction of $\hat{h}$, we have

$$\hat{h}\psi_n(\zeta) = \psi_n(\zeta)E_n, \quad E_n = 2D_0 a \left(n + \frac{1}{2} \right), \quad n = 0, 1, 2, \cdots.$$

Therefore, if the initial condition is

$$C_0(\zeta) = e^{\frac{1}{2}a\zeta^2} \left(\frac{a}{\pi} \right)^{1/4} \psi_n(\zeta), \tag{5.22}$$

the concentration for any time is

$$C(\zeta,t) = e^{-D_0 at} e^{\frac{a\zeta^2}{2}} e^{-2D_0 a \left(n + \frac{1}{2} \right) t} \psi_n(\zeta). \tag{5.23}$$

6. Other Cases

In some cases the diffusion coefficient is given by [5, 10]

$$D(x) = \frac{D_0}{\left(1 + \left[\frac{d}{dx} \left(\sqrt{\frac{A(x)}{\pi}} \right) \right]^2 \right)^{1/2}}. \tag{6.1}$$

When the change of variable (3.2) is invertible, we can study these cases. For instance, for the conical channel, which has cross section $A(x) = \pi(1 + \lambda x)^2$, the change of variable in this case is

$$y = x \left(\frac{\sqrt{1 + \lambda^2}}{D_0} \right)^{\frac{1}{2}}$$

and it is invertible.

7. Summary

We have shown a relation between Fick-Jacobs and Schrödinger equation. When the diffusion coefficient is constant, we have obtained exact solutions for Fick-Jacobs equation for different geometries. Moreover, the general case was studied and it has shown that the solutions of Fick-Jacobs equation can be seen as a quantum state.

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