A Computer Algebra Solution of Ermakov Equation Corresponding to Diffusion Interpretation of Wave Mechanics

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ABSTRACT

It has been long known that a year after Schrödinger published his equation, Madelung also published a hydrodynamics version of Schrödinger equation. Quantum diffusion is studied via dissipative Madelung hydrodynamics. Initially the wave packet spreads ballistically, than passes for an instant through normal diffusion and later tends asymptotically to a sub-diffusive law. In this paper we will review two different approaches, including Madelung hydrodynamics and also Bohm potential. Madelung formulation leads to diffusion interpretation, which after a generalization yields to Ermakov equation. Since Ermakov equation cannot be solved analytically, then we try to find out its solution with *Mathematica* package. It is our hope that these methods can be verified and compared with experimental data. But we admit that more researches are needed to fill all the missing details.

Keywords: quantum hydrodynamics, quantum diffusion, quantum-classical correspondence, Madelung equation, Ermakov equation, computer algebra solution.

1. Introduction

The Copenhagen interpretation of quantum mechanics is guilty for the quantum mystery and many strange phenomena such as the Schrödinger cat, parallel quantum and classical worlds, wave-particle duality, decoherence, collapsing wave function, etc.

The Copenhagen interpretation of QM was challenged not only by Schrödinger but also by a large group of physicists led by Albert Einstein who claimed that the quantum mechanical description of the physical reality cannot be considered complete, as shown in their famous EPR paper Einstein, Podolsky and Rosen. They concluded their derivations by stating that "*While we have thus shown that the wave function does not provide a complete description of the physical reality, we left open the question of whether or not such a description exists. We believe, however that such a theory is possible.*" Einstein did not object to the probabilistic description of sub-atomic phenomena in quantum mechanics. However, he believed that this probabilistic representation was a technique used to overcome the practical difficulties of dealing with a more complicated underlying physical reality, much in the same way he suggested earlier to deal with Brownian motion.

Many scientists have tried, however, to put the quantum mechanics back on *ontological* foundations. For instance, Bohm proposed an alternative interpretation of quantum mechanics, which is able to overcome some puzzles of the Copenhagen interpretation. He developed further the de Broglie pilot-wave theory and, for this reason, the Bohmian mechanics is also known as the de Broglie-Bohm theory.[2]

Long before the Bohmian mechanics proposal, a year after Erwin Schrödinger published his celebrated equation, Erwin Madelung showed (in 1927) that it can be written in a hydrodynamic form. Madelung's representation has a seemingly major disadvantage by transforming the linear Schrödinger equation into two nonlinear ones. Nonetheless, despite of its additional complexity, the hydrodynamic analogy provides important insights with regard to the Schrödinger equation.

In this paper we will review two different approaches, including Madelung hydrodynamics and also Bohm potential. It can be shown that Madelung formulation leads to diffusion interpretation, which after a generalization yields to Ermakov equation. Since Ermakov equation cannot be solved analytically, then we try to find out its solution with *Mathematica* package. It is our hope that these methods can be verified and compared with experimental data.

Nonetheless, we admit that more researches are needed to fill all the missing details, for example we do not yet discuss comparison between quantum trajectories and classical trajectories such as in Wilson chamber experiments.

2. Bohmian quantum potential [2]

The evolution of the wave function of a quantum mechanical system consisting of N particles is supposed to be described by the Schrödinger equation:

$$i\hbar\partial_t\psi = \left(-\frac{\hbar^2}{2m}\nabla + U\right)\psi. \tag{1}$$

The complex wave function can be presented generally in the polar form:

$$\psi = \sqrt{\rho}\exp\left(\frac{iS}{h}\right), \tag{2}$$

Where $\rho = |\psi|^2$ is the N-particles distribution density and $\frac{S}{\hbar}$ is the wave function phase.

Introducing equation (2) into (1) one gets a set of equations:

$$\partial_t\rho = -\nabla.(\rho\nabla S / m), \tag{3}$$

$$\partial_t S + \frac{(\nabla S)^2}{2m} + U + Q = 0, \tag{4}$$

Where quantum potential, Q, is defined as follows:

$$Q = -\frac{\hbar^2}{2m^2}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}. \tag{5}$$

Equation (5) is called Bohmian quantum potential.[2]

3. Madelung quantum potential[2]

If one starts with a different assumption that in equation (3) S is the hydrodynamic-like velocity potential, not the mechanical action as suggested by Bohm, then he can arrives at different relations, such as the two equations proposed by Madelung as follows:

$$\partial_t \rho = -\nabla.(\rho V), \tag{6}$$

$$m\partial V + mV \cdot \nabla V = -\nabla(U + Q), \tag{7}$$

Where

$$V = \nabla S / m. \tag{8}$$

Equations (6) and (7) are known as the Madelung quantum hydrodynamics.[2]

4. Quantum Diffusion and Ermakov equation. Numerical solution

Quantum diffusion is studied via dissipative Madelung hydrodynamics. Initially the wave packet spreads ballistically, than passes for an instant through normal diffusion and later tends asymptotically to a sub-diffusive law. Quantum diffusion (QD) describes a wave packet spreading in a dissipative environment at zero temperature. Since quantum effects are significant for light particles mainly, QD is very essential for electrons, which on the other hand are very important in physics and chemistry. QD has been experimentally observed, however, for muons as well, which are about 200 times heavier than electrons.

Studies on electron transport in solids are strongly motivated by the semiconductor industry, exploring nowadays quantum effects on nano-scale.[4]

Another important transport process affected by quantum effects is the diffusion of hydrogen atoms or molecules in metals and on solid surfaces. The quantum tunneling accelerates the hydrogen diffusion, which is essential for many modern technologies for storage and use of hydrogen as a fuel, chemical reagent, etc.[4]

Now, we start with Madelung equations (6)(7)(8), then introducing now both expressions for ρ and V in Eq. (7) yields the following equation:[4]

$$m\partial_t^2\sigma + b\partial_t\sigma = \frac{\hbar^2}{4m\sigma^3},$$

(9)

describing the evolution of the root-mean-square displacement σ. Introducing new dimensionless dispersion and time parameters, Eq. (9) acquires the universal form of a dissipative Ermakov equation:

$$\partial_\tau^2\xi + \partial_\tau\xi = \xi^{-3},$$

(10)

where

$$\xi^2 \equiv \frac{2b\sigma^2}{\hbar}$$

(11)

$$\tau = bt/m.$$

(12)

It is known that such an Ermakov equation cannot be solved analytically. In reference [4], solutions have been obtained for some limiting cases. Now we will try to find numerical solution using *Mathematica* package using NDSolve, as follows:[8]

A. Method 1: $\omega(t)$ as a triangle function

```
w[t_]=UnitTriangle[t]

ODE=x''[t]+w[t]^2*x[t]-1/x[t]^3==0;

sol=NDSolve[{ODE,x[0]==1,x'[0]==1},x[t],{t,-10,10}]

Plot[x[t]/.sol,{t,-10,10}]
```

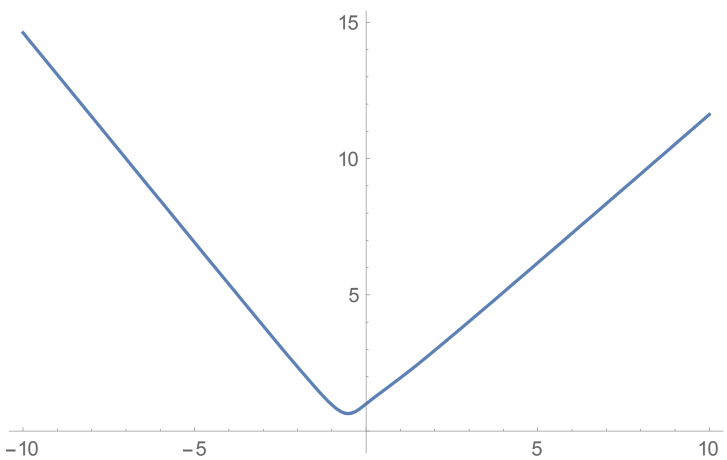

Figure 1. Plot for numerical solution of Ermakov equation, Method 1

B. Method 2: $\omega_2(t)=\omega_1(1+\sin^2(\omega_2 t))$

```
w[t_]=w1*(1+Sin[w2*t]^2);

w1=1;w2=2;

ODE=x''[t]+w[t]*x[t]-1/x[t]^3==0;

sol=NDSolve[{ODE,x[0]==1,x'[0]==1},x[t],{t,-10,10}];
```

Plot[x[t]/.sol,{t,-10,10}]

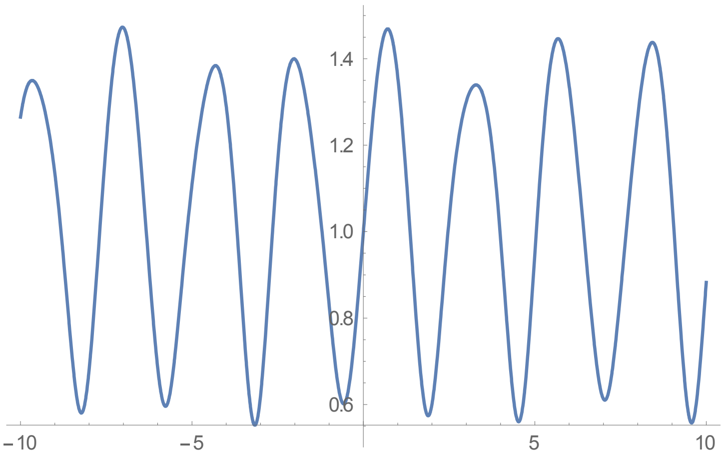

Figure 2. Plot for numerical solution of Ermakov equation, Method 2

5. Discussion and Concluding Remarks

We have discussed five different approaches of describing quantum potential, including Madelung hydrodynamics and also Bohmian mechanics approach of QM. In the last section we solve numerically Ermakov equation corresponding to Madelung diffusion QM using *Mathematica* package. It is our hope that these methods can be verified and compared with experimental data. But we admit that more researches are needed to fill all the missing details.

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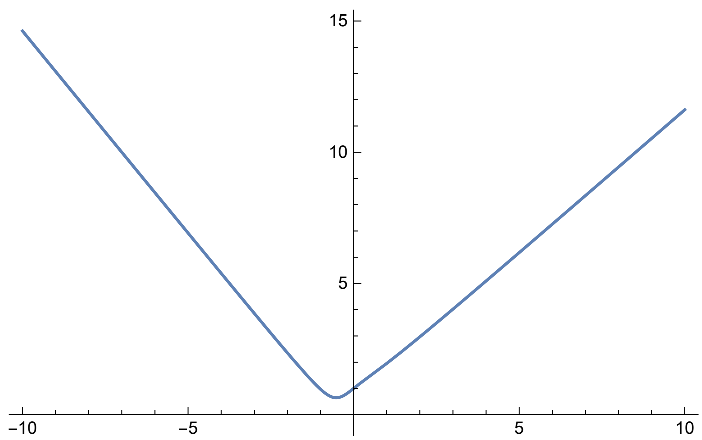
[8] https://mathematica.stackexchange.com/questions/144829/how-to-approach-the-numerical-solution-of-the-ermakov-pinney-equation/144831#144831

In[1]:=
```
w[t_] = UnitTriangle[t]

ODE = x''[t] + w[t]^2 * x[t] - 1/x[t]^3 == 0;

sol = NDSolve[{ODE, x[0] == 1, x'[0] == 1}, x[t], {t, -10, 10}]

Plot[x[t] /. sol, {t, -10, 10}]
```

Out[1]=
```
UnitTriangle[t]
```

Out[3]=
```
{{x[t] → InterpolatingFunction[ Domain: {{-10., 10.}} Output: scalar ][t]}}
```

Out[4]=



In[5]:=

```
w[t_] = w1 * (1 + Sin[w2 * t] ^ 2);

w1 = 1; w2 = 2;

ODE = x''[t] + w[t] * x[t] - 1 / x[t] ^ 3 == 0;

sol = NDSolve[{ODE, x[0] == 1, x'[0] == 1}, x[t], {t, -10, 10}];

Plot[x[t] /. sol, {t, -10, 10}]
```

Out[9]=