A Non-Linear Schrödinger Equation Used to Describe Friction

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ABSTRACT. The energy of a system is defined precisely. A non-linear Schrödinger equation accounting for friction is thereafter presented. The equation could be of importance in nano-technology where friction problems abound. The solutions are for special cases of the harmonic oscillator examined numerically. The solution is shown numerically to approach the stationary zero-point solution of the conventional Schrödinger equation when time approaches infinity.
KEYWORDS. Differential equations, Schrödinger equation, quantum mechanics, energy, wave function

1 Introduction

Sliding friction has been studied macroscopically for several hundred years, and is one of the oldest and most important problems from a practical point of view. The ability to produce durable low-friction surfaces has become an important factor in the miniaturization of moving components in many technological devices [1], but in some cases one wants to maximize the friction rather than to minimize it. Without friction it would be impossible to walk or to drive a car. Also during fast compression of explosives by impact, the friction between microscopic grains creates hot areas causing the explosive to ignite [2],[18].

The classical and quantum mechanical analyses of systems in general share the property of symmetry when time changes direction. This time symmetry relates to the possibility of formulating the fundamental equations of Nature by using the Lagrangian approach. Thus an exact treatment of the fundamental equations appears to dispense with the use of friction forces, since friction forces involve time asymmetry. An exact treatment of the fundamental equations for large objects is, of course, a very complicated mathematical problem, and the introduction of the concept of friction has been a convenient way of avoiding the complications associated with an exact microscopic mathematical approach.

Friction arises from the transfer of collective translational kinetic energy into nearly random motion, and can formally be considered as resulting from the process of eliminating, classically or quantum mechanically, the microscopic degrees of freedom in a systematic manner. Accounting for the microscopic degrees of freedom, the standard algorithm within the quantum mechanical approach is to construct an effective quantum mechanical field theory. Our approach is different. We assume that the microscopic degrees of freedom are integrated out classically, and that the classical equation is given to us as an equation involving friction. Given the existence of this classical differential equation, a way of constructing the corresponding quantum mechanical equation is provided. Of course, this new equation must in some limit approach the classical equation, using some appropriate correspondence principle. Surprisingly, a direct way of constructing the equation is found. The constructed non-linear quantum mechanical equation should be of interest in the field of nano-technology where friction is very important to control [1]. Of special interest are situations where small objects (e.g. atoms and molecules) interfere with larger objects (e.g. macroscopic surfaces)[3], probably stressing a quantum mechanical approach for the smaller object.

Instead of providing examples from the field of nano-technology, the first focus in this article is on the classical and quantum mechanical energy concept, which from our point of view is imprecise, causing problems in the construction of quantum field equations. Different re-normalization techniques are introduced to compensate for the imprecise definition. Many of the problems are indeed solved, but not all of them, which await future study. By first focusing on the classical energy concept, a line of arguments is constructed, and by following the same line of thoughts for the quantum mechanical systems, a precise energy definition is constructed. It is found that both the so-called zero point energy and the arbitrary constant always following the classical potentials are cancelled out and do not contribute to the energy.

Although the studies of the non-linear modifications of the Schrödinger equation are not new [4]-[14], handling friction in association with the Schrödinger equation has to our knowledge not been done. The numerical solutions of the proposed non-linear Schrödinger friction equation are, as illustrated with some examples for the harmonic oscillator, shown numerically to approach the stationary zero-point solution of the conventional Schrödinger equation when time goes to infinity. This seems very natural since it is expected that friction reduces the energy of the solution, causing an expected threshold at the corresponding zero-point solution.

Section 2 discusses the classical energy concept, proposing a classical energy definition. Section 3 presents the non-linear Schrödinger equation with friction, supplemented with the quantum mechanical energy definition. Section 4 shows various numerical examples of the equation. Section 5 concludes.

2 The classical energy

Assume as an example that the classical equation is given by the harmonic oscillator, i.e.[1]

$$\ddot{N}(t) \overset{mod}{=} -N(t), \quad \forall t, \tag{2.1}$$

where N(t) is position and "mod" means model assumption. To find the energy $e(t)$ of this system at time t, the literature provides the following quantity,

[1] We chose units such that the mass is one and the frequency is 1.

$$
\begin{aligned}
& \overset{def}{e_l(t)} = e_k(t)+e_p(t)=(1/2)\dot{N}(t)^2+(1/2)N(t)^2 \\
& \Rightarrow \quad \dot{e}_l(t)=\dot{N}(t)\,\ddot{N}(t)+N(t)\,\dot{N}(t) \\
& =\dot{N}(t)\left(\ddot{N}(t)+N(t)\right)=0, \quad \overset{def}{e_k(t)} = (1/2)\dot{N}(t)^2, \\
& \overset{def}{e_p(t)} = (1/2)N(t)^2 \quad \forall t,
\end{aligned}
\tag{2.2}
$$

where "def" means definition and $e_l(t)$ is a constant through time (also called a constant of motion). $e_k(t)$ is called the kinetic energy and $e_p(t)$ is called the potential energy. A measurement of the energy of the system should give the energy $e_l(t)$, but there are of course other constants through time that a measuring process in principle could reveal, e.g.

$$
\overset{mod}{e_a(t)} = (1/2)\dot{N}(t)^2+(1/2)N(t)^2+a \quad \forall t, \tag{2.3}
$$

where the constant a is arbitrary. If the empiricism rules out other possibilities implying $e(t)=e_l(t)$, which we refer to as the classical result, and ad-hoc postulate of the nullity of the constant must be provided. In order to reduce the number of axioms as much as possible, and at the same time searching for a mechanism that could give a unique energy for a given equation of motion, the following procedure to measure the energy is proposed:

Assume that the process of measuring means to impose an interaction between the system and the measuring device, where the interaction is described by friction, i.e. substituting (2.1) with

$$\ddot{N}_m(t) \overset{mod}{=} -N_m(t) - \varepsilon \dot{N}_m(t), \quad t \geq t_m, \tag{2.4}$$

where ε is a constant and the measurement starts at time t_m. Thus (2.4) applies for the system after the measuring process is started. Define the energy by

$$\begin{aligned} e_m(t_m) &\overset{def}{=} -\int_{t_m}^{\infty} \left(\ddot{N}_m(t) + N_m(t)\right) \dot{N}_m(t) dt \\ &= -\left[(1/2)\dot{N}_m(t)^2 + (1/2) N_m(t)^2 \right]_{t_m}^{\infty} \\ &= (1/2)\dot{N}_m(t_m)^2 + (1/2) N_m(t_m)^2 \\ &= e_l(t_m), \quad \lim_{t\to\infty} N_m(t) = 0. \end{aligned} \tag{2.5}$$

The result of the integration from t_m to infinity is almost independent of the exact nature of the measuring process since result follows as long as $\lim_{t\to\infty} N(t) = 0$. Also the result is independent of the time t_m for the start of the measuring process in this example where the force is only dependent on N(t).

The general algorithm for finding the classical energy of a system at time t can now be constructed. Assume that in general the equation of motion is given as

$$\ddot{N}(t) \overset{mod}{=} f\left(N(t)\right) \quad \forall t. \tag{2.6}$$

The measuring process involving linear friction is described by

$$\ddot{N}_m(t) \overset{mod}{=} f\left(N_m(t)\right) - \varepsilon v_m(t), \quad \dot{N}_m(t) = v_m(t), \quad t \geq t_m. \tag{2.7}$$

The energy at time t_m is then given by

$$\begin{aligned} e_m(t_m) &\overset{mod}{=} -\int_{t_m}^{\infty}\left[\ddot{N}_m(t) - f\left(N_m(t)\right)\right]\dot{N}_m(t)dt \\ &= -\left[(1/2)\dot{N}_m(t)^2 + V\left(N_m(t)\right)\right]_{t_m}^{\infty} \\ &= (1/2)\dot{N}(t_m)^2 - \left[V\left(N_m(t)\right)\right]_{t_m}^{\infty}, \quad \underset{t\to\infty}{Lim}\,\dot{N}_m(t) = 0, \\ DV(n) &\overset{def}{=} -f(n), \quad N_m(t_m) = N(t_m), \end{aligned} \tag{2.8}$$

where "D" means derivative with respect to the position n. Observe that the energy is independent of t_m, i.e. $\dot{e}_m(t_m) = 0, \quad \forall t_m$. This means that the measurement process of the energy completely eliminates the energy so that it equals zero after completion of the measurement process. (This does of course not mean that a classical measurement process of something else than energy (e.g. momentum, position), completely eliminates the energy after completion of the measurement process.) The arbitrary constant of the potential $V(n)$ is now cancelled out, but still the energy $e_m(t_m)$ is ill posed if the potential happens to be singular such that $\underset{t\to\infty}{Lim} V\left(N_m(t)\right) = 0$ does not exist.

The energy in (2.8) can in general be defined also for a system where the force depends on the rates. Thus we in the most general case provide

$$\begin{aligned} e_m(t_m) &\overset{mod}{=} -\int_{t_m}^{\infty}\left[\ddot{N}_m(t) - f\left(N_m(t), \dot{N}_m(t)\right)\right]\dot{N}_m(t)dt, \\ \underset{t\to\infty}{Lim}\,\dot{N}_m(t) &= 0, N_m(t_m) = N(t_m), \end{aligned} \tag{2.9}$$

Although integrating the path after the interaction between the system and the measuring device gives the proposed measurement of the energy, the energy left after the measurement is zero. So in this respect a classic measurement of the energy is very different from a measurement of the position.

The classical position can be measured without destroying or interfering with the position.

3 The quantum energy

Introducing[2]

$$\psi(t,n) \overset{def}{=} \rho(t,n)^{1/2}\, Exp[i\, s(t,n)], \quad D\, s(t,n) \overset{def}{=} v(t,n) \tag{3.1}$$

and inserting into the familiar Schrödinger equation gives the de Broglie version of the Schrödinger theory [4], to read

$$\begin{aligned} &\dot{v}(t,n)+v(t,n)D\Big(v(t,n)\Big)=f(n)+(1/2)D\Big[\Big(D^2\rho(t,n)^{1/2}\Big)\Big/\rho(t,n)^{1/2}\Big], \\ &\dot{\rho}(t,n)+D\Big(\rho(t,n)v(t,n)\Big)=0, \end{aligned} \tag{3.2}$$

where the classical system is given by (2.6).

We propose the following two criteria as the most plausible to design a quantum system that best corresponds to the classical system with linear friction in (2.7). The first criterion is the expectation equation

$$\ddot{E}(N)=E\Big(f(N)\Big)-\varepsilon E\Big(v(t,N)\Big), \quad \dot{E}(N)=E\Big(v(t,N)\Big), \tag{3.3}$$

where "E(·)" means expectation value. We believe that equation (3.3) is one of the basic relations that a quantum equation should fulfil. A second and more obvious criterion is that $\rho(t,n)$ is a proper density function fulfilling the standard criteria of weak positivity and integration to one. We thus propose the quantum system

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[2] We have chosen unit such that $m=1, \hbar=1$

$$\dot{v}(t,n)+v(t,n)D(v(t,n) \overset{mod}{=} f(n)-\varepsilon\ v(t,n)+ (1/2)D\left[\left(D^2\rho(t,n)^{1/2}\right)/\rho(t,n)^{1/2}\right], \quad (a) \qquad (3.4)$$

$$\dot{\rho}(t,n)+D(\rho(t,n)v(t,n) \overset{mod}{=} 0, \quad (b)$$

where the friction term or velocity term $-\varepsilon v_m(t)$ in (2.7) is substituted by $-\varepsilon v(t,n)$. It is easily shown by using (3.4a) and (3.4b) that (3.3) follows. Multiplying (3.4) with $\rho(t,n)$, integrating by parts, applying the identity relation

$$\begin{aligned} &h(t,n)(1/2)D\left[\left(D^2h(t,n)^{1/2}\right)\Big/h(t,n)^{1/2}\right] \\ &=(1/4)D\left[D^2h(t,n_1)-\left(Dh(t,n)\right)^2\Big/h(t,n)\right], \end{aligned} \qquad (3.5)$$

where $h(\cdot)$ is an arbitrary function, subsequent integration and application of the boundary conditions

$$D^2\rho-\left(D\rho\right)^2\Big/\rho=0 \quad \textit{at boundaries}, \qquad (3.6)$$

imply (3.3). Using (3.1), one integration of (3.4) gives

$$\begin{aligned} &-(1/2)D^2\psi(t,n)+V(n)\psi(t,n)+\varepsilon\,(1/(2i)) \\ &\times Log\left[\psi(t,n)/\psi(t,n)^*\right]\psi(t,n)=i\,\dot{\psi}(t,n), \end{aligned} \qquad (3.7)$$

which is the crucial equation of this article, hereafter referred to as the non-linear Schrödinger friction equation, or the quantum friction equation [15].[3] Observe the extra non-linear "friction" term $\varepsilon(1/(2i))Log\left[\psi(t,n)/\psi(t,n)^*\right]\psi(t,n)$ in (3.7) compared with the conven-

[3] In (3.7) Log means the principal value or principal branch of the logarithm where the phase is between minus Pi and plus Pi [16, page 63]. When the denominator $\psi(t,n)^*$ in the logarithm in (3.7) equals zero, then we define the logarithm multiplied with $\psi(t,n)$ to be equal zero.

tional Schrödinger equation. Although one may theoretically think of many ways of adding friction terms to the Schrödinger equation so that it reduces to the standard Schrödinger equation in spezial circumstances (when friction approaches zero), we believe that our proposal is the most plausible one for linear friction. We do not claim that equation (3.3) together with the classical equation uniquely determine (3.4). But, by focusing on Poincaré's [17] criteria for mathematical theory, symmetry, harmony, balance, we believe that (3.4) is the most plausible choice. Of course, empirics will over time terminate all discussion. Observe that the classical friction equation which was linear, gives a non-linear quantum mechanical term. Our numerical examples in the next section show for the harmonic oscillator that the solutions of (3.7) asymptotically approach the stationary zero-point solutions of the conventional Schrödinger equation when time t approaches infinity.

We now proceed to measure the energy of the quantum system. Before the measurement is started, the following expected energy is a constant thorough time, i.e.

$$\bar{e}(t) = \int_{-\infty}^{\infty} \psi(t,n)^* \left(-(1/2)D^2\psi(t,n) + V(n)\psi(t,n)\right) dn. \tag{3.8}$$

The classical potential $V(n)$ is only given at a constant near, so therefore the equation in (3.8) does not give a unique value. In order to define the energy precisely, the same lines of thoughts as in the classical situation are followed. Assume that the measurement starts at time t_m. Thereafter the friction equation (3.7) is descriptive, and the released energy is given by

$$\bar{e}_m(t_m) \overset{def}{=} -\left[\int_{-\infty}^{\infty} \psi_m(t,n)^* \left(-(1/2)D^2\psi_m(t,n) + V(n)\psi_m(t,n)\right) dn\right]_{t_m}^{\infty}, \tag{3.9}$$

where $\psi_m(t,n)$ satisfies the friction equation (3.7). Assuming that the solution $\psi_m(t,n)$ approaches a stationary solution when time approaches infinity, which is likely to be the stationary zero-point solution if it exists gives that

$$\begin{aligned} \bar{e}_m(t_m) &= \int_{-\infty}^{\infty} \psi_m(t_m,n)^* \left(-(1/2)D^2\psi_m(t_m,n) + V(n)\psi_m(t_m,n)\right) dn - e_0 \\ &= \bar{e}(t_m) - e_0, \end{aligned} \tag{3.10}$$

where

$$e_0 \overset{def}{=} \lim_{t\to\infty} \int_{-\infty}^{\infty} \psi_m(t,n)^* \left(-(1/2)D^2\psi_m(t,n)+V(n)\psi_m(t,n)\right) dn. \quad (3.11)$$

Using the approach in this section, both the zero-point energy e_0 in equation (3.11) and the arbitrary constant of the potential is cancelled out for the expected energy $\bar{e}_m(t_m)$. In order to have a well-posed description the limit $\lim_{t\to\infty} \int_{-\infty}^{\infty} \psi_m(t,n)^* \left(-(1/2)D^2\psi_m(t,n)+V(n)\psi_m(t,n)\right) dn$ must exist.

4 Simulations and comparisons

This section compares the quantum equations with and without friction for various scenarios. The initial probability densities are as examples given by Gaussian distributions of the form

$$\rho(t_0,n) = (2\pi\sigma^2)^{-1/2} e^{-(n-a)^2/(2\sigma^2)}, \quad v(t_0,n) = 0, \quad a = constant, \quad (4.1)$$

or as a sum of two initial Gaussian distributions of this form. The analytical solution of the Schrödinger equation is for one initial Gaussian distribution given as

$$\begin{aligned}
\psi(t,n) &= (i)^{-1/2}(2\pi\sigma^2)^{-1/4}\sigma^{1/2}\left\{\left(i\sigma Cost + Sint/(2\sigma)\right)\Big/\left(\sigma^2 Cos^2 t + 1/(4\sigma^2)Sin^2 t\right)\right\}^{1/2} \\
&\quad \times Exp\Big[-(n-aCost)^2(1+i2\sigma^2 Cost/Sint)/\{4[\sigma^2 Cos^2 t + 1/(4\sigma^2)Sin^2 t]\} \\
&\quad + i(n-aCost)^2 Cost/(2Sint)\Big], \quad t_0 = 0, \\
s(t,n) &= (1/2)(n-aCost)^2 Cost\left(1/(4\sigma^2)-\sigma^2\right)Sint\Big/[\sigma^2 Cos^2 t + 1/(4\sigma^2)Sin^2 t], \\
v(t,n) &= Ds(t,n), \\
\rho(t,n) &= \psi(t,n)^*\psi(t,n) \\
&= (2\pi)^{-1/2}\left(\sigma^2 Cos^2 t + (4\sigma^2)^{-1}Sin^2 t\right)^{-1/2} e^{-(n-aCost)^2/[2(\sigma^2 Cos^2 t + (4\sigma^2)^{-1}Sin^2 t)]}.
\end{aligned} \quad (4.2)$$

Inserting a=0 and $\sigma = 2^{-1/2}$ into (4.2) gives the so-called zero-point stationary solution. The variance is $\sigma^2 = 1/2$. Two different values of a will be used. For two initial Gaussian distributions it follows from the linearity of the Schrödinger equation that the solution is given as the average of the wave functions corresponding with the two initial values of a.

Stationary solutions of the friction equation (3.7) are found by setting $\dot{\psi}(t,n) = 0$ in (3.7), and classes of stationary solutions are found by

$$\left[\psi(n)/\psi(n)^*\right] = const, \quad i.e.\ \psi(n) = \rho(n)^{1/2}\, Exp[i\, b], \quad b = constant. \tag{4.4}$$

Defining $\varepsilon b = -e_i$, inserting (4.4) into (3.7) gives

$$-(1/2)D^2\left(\rho(n)^{1/2}\right) + V(n)\rho(n)^{1/2} = e_i\rho(n)^{1/2}. \tag{4.5}$$

Observe that the proposed classes of stationary solutions of the non-linear Schrödinger friction equation (3.7) also are solutions of the conventional Schrödinger equation.

Fig. 4.1 shows the square root of the variance (Stand) as functions of time (Time) for tree different cases denoted as A, B, C. The expectations are zero at all times in all cases.

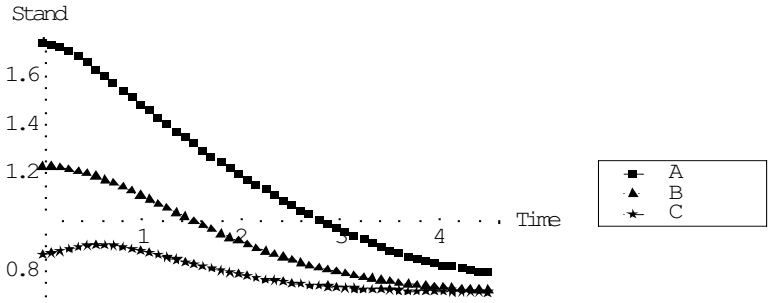

Fig. 4.1. Different standard deviations as functions of time t, a=0, $\varepsilon = 4.0$ in all cases. A: Stand(0) $= \sigma = 1.73$,
B: Stand(0)= $\sigma = 1.22$, C: Stand(0)= $\sigma = 0.87$.

The quantum solutions in the figure are found by solving (3.7) numerically. These solutions approach a limit equal to the stationary variance

σ^2 =0.5, i.e. Stand= $\sqrt{0.5} = 0.71$ (commented in the text after equation (4.2)) as time t approaches infinity. The limit density function $\lim_{t\to\infty} \rho(t,n)$ seems to have a Gaussian form, and is always the same for all initial conditions.

Fig. 4.2 shows the density $\rho(t,n)$ without friction (ε=0) referred to as Sim1 as a function of time t and position n.

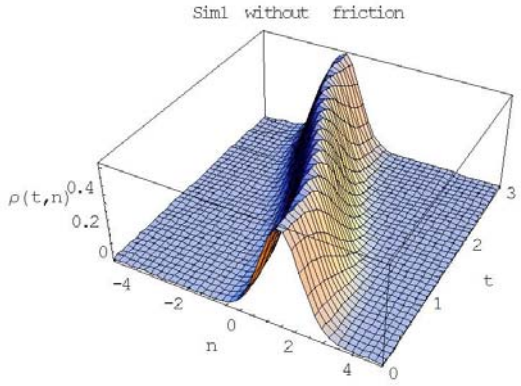

Fig. 4.2: Quantum solution without friction as a function of time,

$$\sigma^2 = 1/2, a = 1.5, \varepsilon = 0 .$$

The variance σ^2 in Fig. 4.2 stays stable through time. The solution is found numerically, but equation (4.2) can also be used directly.

Changing from a=1.5 to a=-1.5 to generate the mirror solution (i.e. starting to the left rather than to the right), Fig. 4.3 shows the density $\rho(t,n)$ without friction referred to as Sim2 when $\sigma^2 = 1/2, a = -1.5, \varepsilon = 0$.

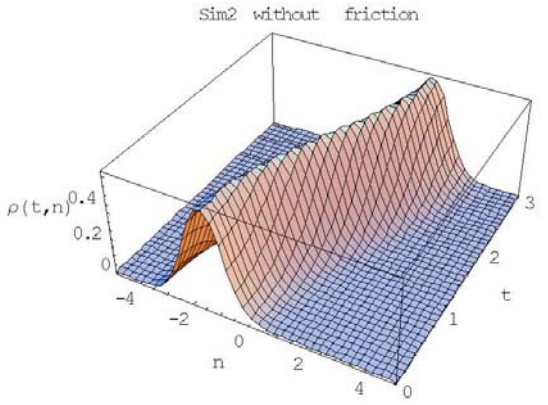

Fig. 4.3: Quantum solution without friction as a function of time,

$$\sigma^2 = 1/2, a = -1.5, \varepsilon = 0 .$$

Fig. 4.4 shows the average of the two mirror solutions in Figs. 4.2 and 4.3, referred to as (Sim1+Sim2)/2. (Note that the average of the densities $\rho(t,n)$ is plotted and not the squared average of the two wave functions $\psi(t,n)$.) This is not an exact solution.

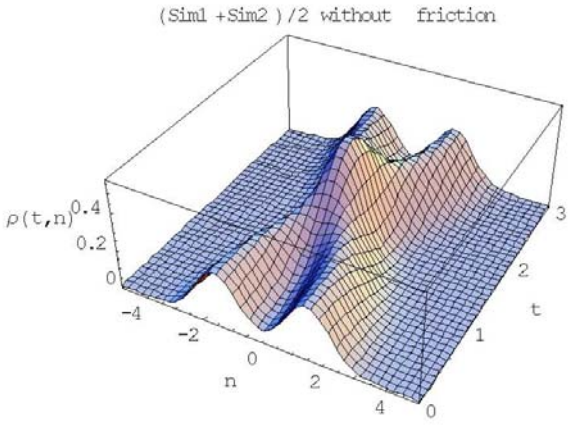

Fig. 4.4: The average solution (Sim1+Sim2)/2 without friction of the two initial Gaussian distributions as a function of time.

$$\sigma^2 = 1/2, Abs(a) = 1.5, \varepsilon = 0 .$$

Fig. 4.5 shows the quantum solution as a function of time using the two initial Gaussian distributions.

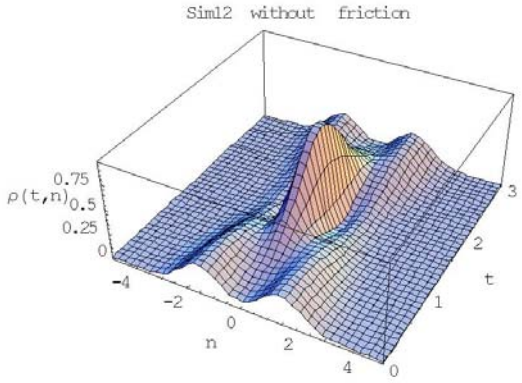

Fig. 4.5: Quantum solution without friction as a function of t,

$\sigma^2 = 1/2, Abs(a) = 1.5, \varepsilon = 0$.

Observe the difference between the average solution in Fig. 4.4 and the quantum solution in Fig. 4.5. The interference pattern is clearly visible in the quantum solution in Fig. 4.5. Fig. 4.6 shows the quantum solution with the two initial Gaussian distributions with friction with the magnitude of ε=4.0, is found by solving (3.7) numerically.

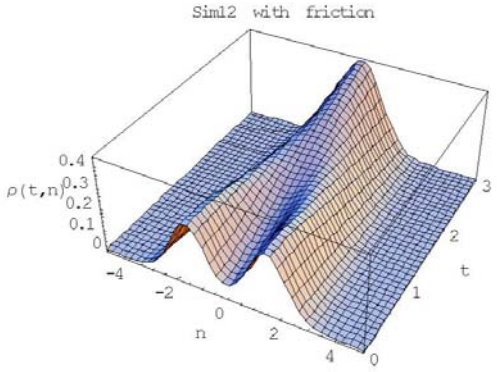

Fig. 4.6: Quantum solution with friction as a function of time, $\sigma^2 = 1/2, Abs(a) = 1.5, \varepsilon = 4.0$.

Observe how the two Gaussian distributions in Fig. 4.6 coalescence when time t increases, in the sense that the density eventually approaches a narrow Gaussian distribution with variance $\sigma^2 = 1/2$. We believe that this effect is caused by the strong non-linearity of the friction equation (3.7). Reducing the magnitude of the friction from ε=4.0 to an arbitrarily small but positive number (e.g. ε=0.01) still causes the density $\rho(t,n)$ to eventually reach a Gaussian distribution with $\sigma^2 = 1/2$ after a sufficiently long time period t. We observe no interference pattern in Fig. 4.6. Fig. 4.6 stands in stark contrast to Fig. 4.5 without friction, where there is an alternating narrowing and broadening of the density through time.

5 Conclusion

A quantum equation with friction is discussed. A precise energy definition is given by first focusing on the classical energy concept. A sequence of arguments is constructed, and by following the same sequence of thoughts for the quantum mechanical systems, a precise energy definition is constructed with the implication that introducing an explicit re-normalization technique is unnecessary. We see especial potential for the non-linear friction equation in the field of nano-technology where friction is important to control. Quantum solutions with friction are for the harmonic oscillator shown numerically to approach the stationary solutions of the conventional Schrödinger equation when time goes to infinity. We believe this to be a general result, although we have not shown this for other processes than the harmonic oscillator.

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