# Modeling the Probability Density Function of an Elastically Bound Particle

Nicholas Anthony Potter

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**Abstract**

The behavior of the probability density function of an elastically bound particle is modelled using the $\theta$-method and a combination of different finite-difference schemes. The issues of each approach are discussed, as are the results of the model for a number of different initial conditions and coefficient equations $p(x)$.

## 1 Introduction

The probability density function of an elastically bound particle on 1-dimension behaves according to the following partial differential equation

$$u_t = Du_{xx} + \gamma(p(x)u)_x \tag{1}$$

on a line between $-L$ and $L$ with boundary conditions

$$Du_x(-L) - \gamma Lu(-L) = 0 \tag{2a}$$
$$Du_x(L) + \gamma Lu(L) = 0 \tag{2b}$$

Here the PDE is modeled using the $\theta$-method finite differences scheme for the equation as a whole. The Thomas Algorithm is used to solve the resulting tridiagonal matrix. A variety of parameters are investigated, focusing especially on the bounds, and examining the behavior of the long-run equilibrium. Of particular interest is a number of different initial conditions, as well as a variety of different definitions for $p(x)$.

## 2 Methodology

Since we are interested in the application of numerical methods and their effectiveness, I describe several different approaches here, each with varying degrees of success. However, before presenting the various methods, lets examine the setting surrounding (1).

To begin with, we want the behavior of the probability density function to behave certain laws; namely, that its sum should always equal 1. From this we can derive our boundary conditions (2a) and (2b), since the sum of the pdf is analogous to the conservation of heat. In this case, we have

$$h_t(t) = \int_{-L}^{L} u_t(x,t)dx = \int_{-L}^{L} Du_{xx} + \gamma(p(x)u)_x \tag{3}$$

which gives

$$(Du_x + \gamma p(x)u)|_{-L}^{L} \tag{4}$$

from which our boundary conditions follow.

A number of numerical schemes were developed in the process of analyzing (1). Three different schemes had notable results, though one of them encapsulates the other two, and so it is focused on here. The use of the $\theta$-method on the diffusion term $Du_{xx}$ is straightforward and presents no problems. However, the first order term $\gamma(p(x)u)_x$presents difficulties under several different schemes. In our initial problem, $p(x) = x$, which presents a problem for using a center difference scheme to approximate $\gamma(p(x)u)_x$ since x changes sign. We can use upwind differencing to approximate the first order term explicitly, using forward differences when $p(x) > 0$, backward differences with $p(x) < 0$, and center differences when $p(x) = 0$. Alternatively, we can extend the $\theta$-method to include the first order term. As a third scheme, we can combine the previous two. We shall see that each oth theseboth of these schemes lead to changing heat values for certain initial conditions and parameters.

Since the use of explicit upwind differencing is similar to using the $\theta$-method with upwind differencing, only the latter is presented here. We use the $\theta$-method to model the entire RHS of the equation, and use forward, backward, and center differences for the first order term depending on $p(x)$. We approximate $u_0$ and $u_J$ by shifting the grid $(1/2)\Delta x$ to the left and taking

a center difference for $u_0$ and $u_J$. From our boundary conditions we then get

$$u_0 = \frac{2D - \gamma L\Delta x}{2D + \gamma L\Delta x} u_1 \tag{5a}$$

$$u_J = \frac{2D - \gamma L\Delta x}{2D + \gamma L\Delta x} u_{J-1} \tag{5b}$$

The Thomas Algorith is used to solve the remaining equations, with $e_0 = k$, where k is the coefficient of $u_0$ in (5a), and $f_0 = 0$. Then we have the following schemes depending on the value of $p(x)$

$$\begin{aligned} -(\theta D\nu + \gamma\omega p_{j+1})u_{j+1}^{n+1} + (1 + \theta(2D\nu + \gamma\omega p_j))u_j^{n+1} - (\theta D\nu)u_{j-1}^{n+1} \\ = (1-\theta)(D\nu + \gamma\omega p_{j+1})u_{j+1}^n + (1 - (1-\theta)(2\nu D - \gamma\omega p_j))u_j^n \\ + (1-\theta)(\nu D)u_{j-1}^n \text{ for } \quad p_j > 0 \end{aligned} \tag{6a}$$

$$\begin{aligned} -(\theta D\nu)u_{j+1}^{n+1} + (1 + \theta(2D\nu - \gamma\omega p_j))u_j^{n+1} - (\theta D\nu - \gamma\omega p_{j-1})u_{j-1}^{n+1} \\ = (1-\theta)(D\nu)u_{j+1}^n + (1 - (1-\theta)(2\nu D + \gamma\omega p_j))u_j^n \\ + (1-\theta)(\nu D + \gamma\omega p_{j-1})u_{j-1}^n \text{ for } \quad p_j < 0 \end{aligned} \tag{6b}$$

$$\begin{aligned} -(\theta D\nu + \gamma\omega p_{j+1})u_{j+1}^{n+1} + (1 + \theta 2D\nu)u_j^{n+1} - (\theta D\nu - \gamma\omega p_{j-1})u_{j-1}^{n+1} \\ = (1-\theta)(D\nu + \gamma\omega p_{j+1})u_{j+1}^n + (1 - (1-\theta)(2\nu D))u_j^n \\ + (1-\theta)(D\nu - \gamma\omega p_{j-1})u_{j-1}^n \text{ for } \quad p_j > 0 \end{aligned} \tag{6c}$$

This scheme can be modified by setting $\theta$ to some value between 0 and 1. If $\theta = 1$then the scheme is fully implicit, and if $\theta = 0$ then the scheme is fully explicit. Also, we obtain a center difference scheme by letting $a$, $b$, $c$, and $d \quad \forall j = 1, 2 \ldots J-1$ equal what they are for $p_j = 0$ above. Of course, we must remember that we have shifted the gridpoints here to obtain our $u_0 and u_J$, so $p_1$ is really $p_{1/2}$.

We will see in the next section how each of these schemes compare. Since the difficulty is in $\gamma(p(x)u)_x$ term, another scheme was tried in which the term was differentiated exogenously, giving us

$$\gamma\Delta t u_j + \gamma p(x)_j \omega(\frac{u_{j+1} - u_{j-1}}{2}) \tag{7}$$

and the $\theta$-method with central differences applied to (7) as well as to our diffusion term. However, this scheme loses all energy extremely quickly, so it is not used extensively here except to examine its maximum condition.[1]

It is important to examine the maximum condition and the error of these schemes, as that may give us some understanding of why they behave as they do. For the scheme above in (7) examining the terms of the entire scheme and rearranging them so that only the $u_j^n + 1$ term is on the left hand side, we get

$$\begin{aligned} & 1 + \gamma\Delta t\theta + 2D\nu\theta \\ & \geq (D\nu\theta + \frac{\gamma\omega p(x)_j}{2}) + (D\nu\theta - \frac{\gamma\omega p(x)_j}{2}) + (1-\theta)((D\nu + \frac{\gamma\omega p(x)_j}{2}) \\ & - (2D\nu + \gamma\Delta t) + (D\nu - \frac{\gamma\omega p(x)_j}{2})) \end{aligned} \tag{8}$$

We can see that this is only satisfied if $\theta \geq \frac{1}{2}$. Also, in order to satisfy that all of the coefficients must be positive, we need $\Delta x \leq \frac{1}{2D\theta}$, which gives us $\Delta t \leq \frac{1}{\gamma - 8D^2\theta^2}$. These restrictions are hardly stringent, and don't seem to yield any useful information. Furthermore, if we conduct an error analysis, we can see that

$$E^{n+1} = \frac{\gamma\Delta t - \theta\gamma\Delta t + 1}{1 + \gamma\Delta t\theta} E^n + \frac{\Delta t}{1 + \gamma\Delta t\theta} \max T^{n+1/2} \tag{9}$$

For $\theta \geq \frac{1}{2}$, we can see that the coefficient of $E^n$ is less than 1, and that the coefficient of $T^n$ is less than 1 for all $\Delta t$ and $\theta$. Thus it would seem that our scheme should be stable as long as we let $\theta \geq \frac{1}{2}$. $h(t)$ is only stable in this scheme if $\theta = .5$, as we will see in the next section.

[1]There is one additional scheme that was developed. This scheme took a $2nd$ centered difference for the wave term. Ironically, though it was for the wrong term for this PDE, the scheme was more stable than any of those presented here, having no fluxuation in $h(t)$. A $2nd$ centered difference was taken of $(p(x)u)_{xx}$. If we think about it, the stability of this scheme should not be suprising, since it is a second term in $u_{xx}$, it exhibits the same stability patterns as the $u_{xx}$ term in our current PDE.

# 3 Results

Each of the three schemes discussed here have different characteristics regarding their stability and points at which they fail. Below I discuss each scheme's ability to model different initial conditions and different functions for $p(x)$. Changing either of these things leads to different behavior in each of the schemes, and lends insight into the strengths and weaknesses of each approach. There are several different initial conditions considered: a uniform distribution $u_j = \frac{1}{\Delta x(J-1)}$for all$j$, a single point distribution $u_j = \frac{1}{\Delta x}$for some$j$ both at the edges and at the center, a triangle distribution with $u_{-L} = 0$, and a cosine function with period $4L$. We also consider $p(x) = x$, $p(x) = x^2$, and $p(x) = \sin(x)$.

We can also speak in general about the behavior of our model, since the three schemes perform similarly in many ways. It is evident from the variety of initial conditions that there are two opposing forces at work in the PDE. Our diffusion term attempts to spread the probability density function over all $x$. On the other hand, our first order term reflects the probability away from the boundaries, pushing it toward the center. The end result of these behaviors in teh long run is a probability distribution that depends on $D$ and $\gamma$. For a more influential $\gamma$, the distribution has a higher peak, while for a more heavily weighted $D$, the distribution is more evenly spread out. These behaviors are true regardless of initial conditions.

In our first scheme, we use center differences to approximate the first order term, and use the $\theta$-method for both terms. This gives us $a_j = \theta(D\nu - \gamma\omega p_{j-1}), b_j = 1 + 2D\theta\nu, \text{and} c_j = \theta(D\nu - \gamma\omega p_{j-1})$. For a uniform initial distribution, we have the long term result seen in (Fig. 1) and the associated $h(t)$ in (Fig. 2). This is quite stable.

We achieve a similar long term solution for an initial distribution at a single point in the middle. However, if we set the initial point near the boundary, we see interesting behavior for $h(t)$, as it spikes to about 1.15 at the beginning, but then converges back to 1. With a triangular intitial condition, we see a wave that approaches from $L$ toward 0 (Fig. 3). Here again $h(t)$ is quite stable.

Our initial conditions fitting a cosine function are not very interesting, since they conform closely to the long term solution anyway, so they are not presented here. However, it is interesting to consider the impacts of varied parameters on the different initial conditions. For $D$ and $\gamma$, we have already discussed their relative effects. By taking $D = .9$ and $\gamma = .1$ we get an

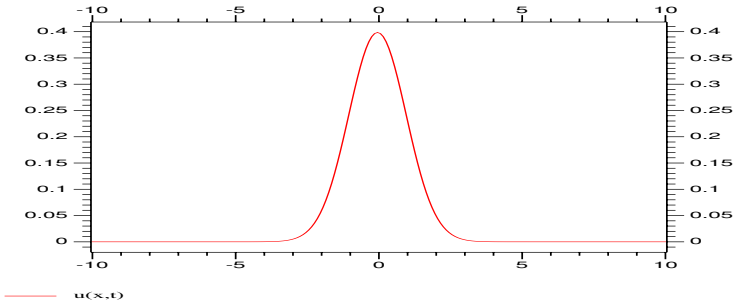


Figure 1: Long term solution for $u(x,t)$, with $D = 1/2$, $\gamma = 1/2$, $\theta = 1$

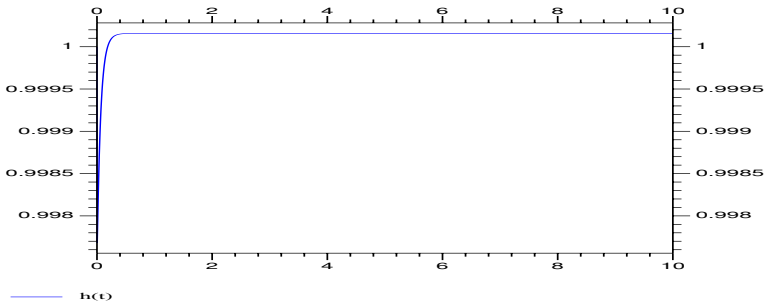


Figure 2: $h(t)$ for $t = 1to10$

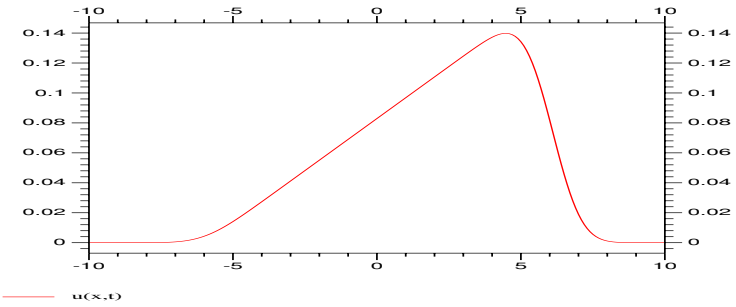


Figure 3: the solution of $u(x, 1)$, with $D = 1/2$, $\gamma = 1/2$, $\theta = 1$

equilibrium solution that is much more dispersed for all x. However, our most interesting results occur when we take $D$ to be small and $\gamma$ large. In this case our method falls apart if our initial conditions are a single point near the boundary, regardless of the value of $\theta$. As we can see in (Fig. 4), we get a wildly out of control oscillation in the side where our initial condition started. Interestingly, we still get $h(t)$ converging to 1 (although it drops to .4 at the beginning). Furthermore it appears that as the probability shifts toward the center the oscillations lessen. If we vary $D$ and $\gamma$,

We get much less stable results with our other schemes. Using upwind differencing for the first-order term without applying the $\theta$-method to it, we get less stable results than in our previous scheme. In (Fig. 5) we can see that $h(t)$ does not stay at 1. Although it initially appears to converge to a new value, if we let $t \geq 2.5$ we can see that it begins to diverge toward 0. By $t = 10$ it is uncertain whether it will begin to converge or whether it will continue toward 0.

If we alter $D$ and $\gamma$, our loss of heat changes. For a high value for $D$ and a low value for $\gamma$, we get very little heat loss. Conversely, for low values of $D$ and high values of $\gamma$, we get much stronger heat loss. However, most importantly for evaluating this scheme, if we let $\gamma = 0$, we see no heat loss

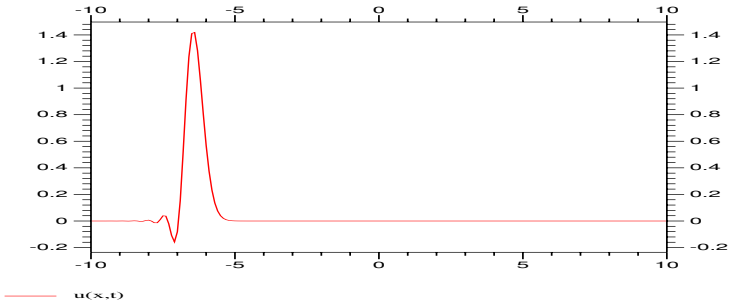


Figure 4: Solution for $u(x,t)$, with $\gamma = .9$, $D = .1$, and $\theta = .5$

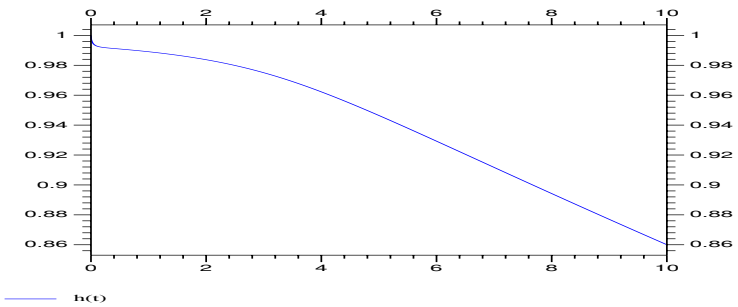


Figure 5: $h(t)$ for $D = .5$ and $\gamma = .5$ and a single midpoint for initial data

regardless of initial conditions or values for $\theta$.

By combining upwind differencing and the $\theta$-method, we hope to get the most stable results, yet in this scheme we get the worst instability in $h(t)$. For the same problem as in (Fig. 5), we see an even larger loss of heat, with no indication that it will converge. This scheme has similar traits to our second scheme, only where we hoped that the $\theta$-method would introduce some stability to the scheme, it has changed little.

Finally, we want to consider the scheme discussed in the last section in which the first order term derivative was taken explicitly and the $\theta$-method with center differences used to model its behavior. Most interestingly, for $\theta > .5$, we see losses in $h(t)$ as time progresses. For $\theta < .5$, we see increases in $h(t)$. However, for $\theta = .5$, $h(t)$ is stable for most initial conditions, failing as the others did when we have a single point near a boundary with $D$ small and $\gamma$ large.

# 4 Discussion

In each of the schemes presented, the first order term is the source of error. If we take $\gamma = 0$ in any of the schemes, we get stable $h(t)$ conditions even for single point near the boundary initial data (though in this case, $h(t) \neq 1$). What remains to be determined then, is why each of the different schemes behaved as they did. Our best results were obtained from the first scheme presented, followed closely by our last scheme, while the two intermediate schemes were dismally worse. Since we originally thought of using the poorly performing upwind differences because $p(x)$ changes sign, we can let $p(x) = x^2$. However, this does not affect the stability of any of the schemesin a positive manner, and actually leads to some larger $h(t)$ variations for our upwind differencing schemes.

Regarding the oscillations that result when our initial conditions are a single point near a boundary, it is likely that we violate the maximum principle here. Physically speaking, getting the system to a point where it could have all the probability at one point near a boundary must be extremely difficult or impossible. We might consider this situation as analogous to approaching absolute 0, or the speed of light, where it takes more and more energy to approach the physical barrier. In this case, our initial condition says that the probability is at that point, but the possibility of getting to that point is near or at 0. Hence there is such a strong force pushing away from the

boundary, while almost no force encouraging the probability density function to spread out. This results in oscillations as the probability is pushed away from the boundary. I have considered the form of our approximation at the near boundaries, but have not been able to derive, beyond this general sense, a mathematical reason for why this occurs.

The use of these different schemes in approximating the behavior of the probability density function of an elastically bound particle has had many suprises in store. I originally intended to examing just one scheme–the one that worked. However, in reality it appears that there often isn't one scheme that works completely. Different schemes may be better at modeling the same system in different ways, for different parameters or initial conditions. Additionally, I expected the explicitly differentiated scheme to be terrible, and considered it just a curiosity. I hardly expected it to perform almost as well as our first scheme (I think it may actually do better in some respects). Furthermore, although we have seen evidence of 'more is not always better' in other schemes (such as a center in time, center in space scheme). I expected the scheme which used the $\theta$-method and upwind differencing to outperform the others. While it didn't do the worst, it wasn't far from it.