UF ETD $\LaTeX 2_\epsilon$ THESIS AND DISSERTATION TEMPLATE TUTORIAL

By

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I dedicate this to everyone that helped revamp this template

ACKNOWLEDGMENTS

Thanks to all the help I have received in writing and learning about this tutorial.

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Abstract of Tutorial Presented to the Graduate School
of the University of Florida in Partial Fulfillment of the
Requirements for the Degree of Master of the Universe

UF ETD LaTeX2ϵ THESIS AND DISSERTATION
TEMPLATE TUTORIAL

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This document is the official tutorial outlining the use and implementation of the UF LaTeX2ϵ template for use on thesis and dissertations. The tutorial will cover the basic files, commands, and syntax in order to properly implement the template. It should be made clear that this tutorial will not tell one how to use LaTeX2ϵ. It will be assumed that you will have had some previous knowledge or experience with LaTeX2ϵ, but, there are many aspects of publishing for the UF Graduate School that requires attention to some details that are normally not required in LaTeX2ϵ.

CHAPTER 1
HOW TO USE THE UF THESIS AND DISSERTATION TEMPLATE

1.1 Introduction

The UF $\LaTeX 2_\epsilon$ thesis and dissertation template is a collection of files that will allow you to produce a document conforming to the standards of the UF Graduate School Editorial Office. We assume that if you're going to use $\LaTeX 2_\epsilon$ to create your thesis or dissertation that you are familiar $\LaTeX 2_\epsilon$ itself. This is not intended to be a tutorial on how to use $\LaTeX 2_\epsilon$ but it is intended to show you how to use $\LaTeX 2_\epsilon$ to create a document that will meet the Graduate School Editorial Office requirements. [8]

The ufthesis.cls file modifies the standard Report Class document to meet the UF Editorial Guidelines. The ufsampleETD.tex file is the main file of your thesis or dissertation. It organizes the order of presentation of the individual files that make up the document. Most of your document will be written in individual files and brought into the document via the `\include{filename}` command. [7]

1.2 Getting Started

There have been no major formatting changes since August, 2006. However, we have made several improvements to the LaTeX Template since then so it's always advisable to work with latest version possible. Download the .zip file that comprises the LaTeX Template and extract the folder containing the template files. Change the name of the folder to avoid any possibility of overwriting your files should you need to re-extract the folder again later in the process. Snir et al. [15]

1.3 Basic Tools Needed

You must have access to an installation of LaTeX. We use MiKTeX (current version is 2.7) and suggest you download and install the complete (approx 500 MB) version rather than the minimal installation. Our template uses several packages in addition to the basic build that are absolutely necessary for it to work. [11]

1.4 MiKTeX

This template assumes that you have MiKTeX 2.5 or later installed on your system. This setup is supposed to auto-install any packages that are called but not already installed as long as you are connected to the Internet. We recommend that if you need to install MiKTeX that you select the complete installation if possible. Tracy and Pecora [16]

1.4.1 Required Files and Programs

To correctly implement the UF ETD LaTeX2ε template in accordance with the UF Gradschool Editorial Office Guildlines. The following files and/or packages are required:

1. MiKTex
2. Some text editor
3. Hanging Package
4. Caption Package
5. Hyperref Package

This is an example of a "short list. Not because there's only 5 items on the list but because each item is less than one line in length. Since short lists are relatively rare the default spacing for the itemize and enumerate environments is for the "long" list where at least one item on the list wraps to a second line. In order to generate a correct short list you need to insert a `\vspace{-10pt}` command after all but the last item on the short list. [10]

The enumerate and itemize environments have been modified to meet Editorial Office guidelines (A special thank you to Antonio Paiva for both the suggestion and the code) but require the ufenumerate.sty file to be in the same folder as your main file. It is loaded via the usepackage{ufenumerate} command. The itemize environment is modified by a set of commands in the usersetcommands file.

1.4.2 Optional Files and Programs

If you need to add a package please remember to place it before the hyperref package in the packages file. Hyperref needs to have several modifications in place to work properly and is essential for the required links. To ensure that it works correctly it must be the last package loaded - and even then it's a delicate operation.

The following programs are not needed but may be very useful when editing documents in LaTeX:

- WinEDT: This text editor is recommended for use editing TeX-files as it has many useful built in macros and is easy to use
- This program can be found and downloaded here: http://www.winedt.com/
- The GIMP (GNU Image Manipulation Program)
  - A freeware graphics editing program for picture editing and file conversions
  - Comparable to Adobe Photoshop
  - Can be downloaded here: http://www.gimp.org/
- A good reference of LaTeX2ϵ commands
  - This should be included on the ETD website here: http://etd.helpdesk.ufl.edu/tex.php

This is an example of "nested" lists. In the itemize environment you can choose an alternative symbol for the "sub-list." The method of specifying this symbol is `\item[-]` where the optional symbol is inserted into the square brackets. Unless you are referring to an item by number, itemized lists are generally preferable to enumerated ones. The difference between itemize and enumerate environments is illustrated by repeating this list below:[9]

1. WinEDT: This text editor is recommended for use editing TeX-files as it has many useful built in macros and is easy to use
2. This program can be found and downloaded here: http://www.winedt.com/
3. The GIMP (GNU Image Manipulation Program)
   (a) A freeware graphics editing program for picture editing and file conversions
   (b) Comparable to Adobe Photoshop
   (c) Can be downloaded here: http://www.gimp.org/
4. A good reference of LaTeX2ϵ commands

(a) This should be included on the ETD website here: http://etd.helpdesk.ufl.edu/tex.html

1.5 Test Compile Before You Start

Make sure you can compile the standard template BEFORE you start putting your content into the files (just to be on the safe side). Since there is little resemblance between the standard TEX Report Class and the ufthesis.cls styles when you latex the ufsampleETD.tex file it will generate several warnings possibly even an error or two. If you latex the file and it stops compiling because of an error press "r" then "enter" and LaTeX will ignore the rest of the errors and warnings. Latex the file again, also pressing "r" and "enter". [12] When all of the warnings are done you can then dvipdfm the file. (Using WinEDT, I just click the dvi - pdf button on the toolbar). This should generate the sampleETD PDF file. As long as you get a PDF in the correct format the errors and warnings generated by LaTeX up to this point are irrelevant. However, if the output at this stage is garbled or non-existent we need to do some troubleshooting: If you've simply unzipped the template and it fails to compile without having made any changes make sure you have the FULL MikTeX installation. There are many LaTeX editors available and almost as many ways to compile a TEX file.

The method we use is to latex filename twice, then dvipdfm filename to create the pdf. Some Editors are more sensitive to errors than others and are unable to bypass the errors. Some others use a different method of compiling the file and can't be re-configured. The template works well on our set-up. If you can't get the template to compile on your machine using the ufthesis.cls file, change the style of the document to the standard report class. Hopefully, you will then at least be able to see the content. Once your content is ready you can come in to the ETD Lab to compile your document in the correct style. [13]

CHAPTER 2
KNOWN ISSUES

2.1 Common Problems

2.1.1 Prime Notation

If you've placed your own content into the template and it fails to compile the most common reason is the use of prime notation in math mode. If you say anything like A' while in the math mode it generates a conflict that will cause the rest of the document to stop compiling. The solution is to use an alternative method of producing the same notation. Replace `A'` with `A^{\prime}` and you will avoid this issue. Since prime notation is quite common we defined a shortcut for this command which allows you to replace `A'` with `A\p`. [4]

2.1.2 Print Scaling

When you print your pdf an often overlooked feature of Adobe Acrobat is the "Print Scaling" feature in the "Page Handling" section of the "Print" dialog box. There are several innocent looking settings that can cause you problems with your first (hardcopy) submission. If you select anything other than "None" the margins and page number locations will be incorrect and could result in your document being rejected without review. [19]. This problem does not exist for the electronic submission but can cause you unnecessary aggravation and expense if you're not careful.

2.1.3 Single Appendix

Since LaTeX numbers everything automatically there is an interesting problem that occurs whenever an author wants to create a document with a single appendix. When this happens, the Editorial Office states that instead of "numbering" the appendix as "A" the word "APPENDIX" should appear in the Table of Contents on the same line as the appendix title without the letter "A." This can be done by suppressing the chapter numbers but then anything that needs to be numbered (Tables, Figures, and/or equations is numbered as a continuation of the previous chapter. This is fine if there's nothing to number, but most of the time this is not the case. [18]

The file appendix.tex is used to control the number of appendices through the counter "noa." Set the value to 1 if there is a single appendix any larger value will work for multiple appendices. If the value is 1 input only appendixA, if the value is two or more allow the other appendices to be input (adding input statements as needed). The beginning of appendixA has another ifthenelse statement regarding the number of appendices and then demonstrates how a landscaped page is inserted as the first page of an appendix. [17]

2.1.4 Decimal Alignment

One of the strangest facts about LaTeX is that it doesn't have a simple method of aligning numbers in a table on the decimal point. The workaround is to create two separate columns align the first to the right and the second to the left and set the separator to a decimal point. This will give the illusion of a decimally aligned column. [5]

Table 2-1. How to align decimals in a numerical column

Category	Result
first	3.14159
second	16.2
third	123.456

As you can see in Table 2-1 the result is an illusion of a decimally aligned column exactly as preferred by the Editorial Office. If done carefully nobody will ever know your dirty secret!

2.2 Long (and/or Wide) Tables

Another problem in LaTeX is the inability to handle long tables. While there are some packages that address this problem none of them quite fit the Editorial Office guidelines. The caption is not repeated but we do need "Table x-y. Continued" on each subsequent page and a repeat of the column headings on each page as well. The following table is the best example of the correct format I can produce. The disadvantage of this method is that much of it is manually set up and changes in the text will cause changes in the table. [14]

For example, at one time the following table was perfectly positioned at the beginning of a page - right after a full page of text. Now the footnote appears on the page with text that is two full pages before the footnote mark! For best results avoid the use of footnotemark and footnotetext commands and try to keep your footnotes outside of floats whenever possible.

2.3 Images That Do Not Show

If you're trying to use the package psfrag you must change the method of compilation for it to render your images correctly. In the main file, change dvipdfm to dvips. Make this same change in the packages file with both the graphix and hyperref package options. You then must compile in the folowing manner:

1. latex filename
2. latex filename
3. bibtex filename (if needed)
4. latex filename
5. latex filename (these latex commands are only needed if the bibtex command was used)
6. dvips filename
7. ps2pdf filename

This can still have a negative effect on the hyperref package and result in broken links and/or incorrect margins in the TOC, LOT and LOF.

[1] This is a test of the emergency footnote network - this is only a test

Table 2-2. Feasible triples for highly variable Grid, MLMMH.

Time (s)	Triple chosen	Other feasible triples
0	(1, 11, 13725)	(1, 12, 10980), (1, 13, 8235), (2, 2, 0), (3, 1, 0)
2745	(1, 12, 10980)	(1, 13, 8235), (2, 2, 0), (2, 3, 0), (3, 1, 0)
5490	(1, 12, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
8235	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
10980	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
13725	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
16470	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
19215	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
21960	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
24705	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
27450	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
30195	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
32940	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
35685	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
38430	(1, 13, 10980)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
41175	(1, 12, 13725)	(1, 13, 10980), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
43920	(1, 13, 10980)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
46665	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
49410	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
52155	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
54900	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
57645	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
60390	(1, 12, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
63135	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
65880	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
68625	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
71370	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
74115	(1, 12, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
76860	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
79605	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
82350	(1, 12, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
85095	(1, 12, 13725)	(1, 13, 10980), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
87840	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
90585	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
93330	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
96075	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
98820	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
101565	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
104310	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
107055	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
109800	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
112545	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)

Table 2-2. Continued

Time (s)	Triple chosen	Other feasible triples
115290	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
118035	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
120780	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
123525	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
126270	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)
129015	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
131760	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
134505	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
137250	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
139995	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
142740	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
145485	(1, 12, 16470)	(1, 13, 13725), (2, 2, 2745), (2, 3, 0), (3, 1, 0)[1]
148230	(2, 2, 2745)	(2, 3, 0), (3, 1, 0)
150975	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
153720	(1, 12, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
156465	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
159210	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
161955	(1, 13, 16470)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)
164700	(1, 13, 13725)	(2, 2, 2745), (2, 3, 0), (3, 1, 0)

CHAPTER 3
REFERENCES

3.1 Manually

You can do your citations and references in LaTeX manually. However, if you do, you lose one of the top reasons for using LaTeX in the first place. Create a bibliography.tex file using the ufsampleETD.bbl file as a guide and include it using the `\include{bibliography}` command. NOTE: This method will not allow you to adjust the format of your bibliography by changing the .bst file called in the main document.

3.2 BibTeX

We use the package natbib in the template. [6] It is used by a large number of journals and offers the widest variety of citation and reference listing options with the least amount of overhead and/or complexity. Determine whether you prefer numbered or un-numbered reference listing. Go to the packages.tex file and make sure your preference is uncommented. Comment (or delete) the other option and you're ready to select a bibliography style.[1] This is done with the `\bibliographystyle{bibstyle}` command. We have included several basic reference styles(the .bst file types). The differences are noted in the following list. Note that the plain style does not change in the either the numbered or author-yearnumbers. [2]

- Numbered References (using the numbered, sort and compress natbib option)
  - plain: numbered citations-brackets, numbered reference list in alphabetical order, full first name last name.
  - ufinit: numbered citations-brackets, numbered reference list in citation order, initials and last name.
  - plainnat: numbered citations-brackets, numbered reference list in alphabetical order, full first name last name.
  - abbrvnat: numbered citations-brackets, numbered reference list in alphabetical order, initials and last name.
  - unsrtnat: numbered citations-brackets, numbered reference list in citation order, full first name last name.

- chicagoReedWeb: numbered citations-brackets, numbered reference list in alphabetical order, last name, full first name.
- apa-good: numbered citations-brackets, numbered reference list in alphabetical order, last name, first and middle initials.

- Un-numbered References (using the authoryear natbib option)
  - plain: numbered citations-brackets, numbered reference list in alphabetical order, full first name last name.
  - ufinit: numbered citations-parentheses, numbered reference list in citation order, initials and last name.
  - plainnat: author-year citations-brackets, un-numbered reference list in alphabetical order, full first name, last name.
  - abbrvnat: author-year citations-brackets, un-numbered reference list in alphabetical order, initial first name, last name.
  - unsrtnat: author-year citations-brackets, un-numbered reference list in citation order, initial first name, last name.
  - chicagoReedWeb: author-year citations-parentheses, un-numbered reference list in alphabetical order, last name, first name, line replaces repeated author.
  - apa-good: author-year citations-parentheses, un-numbered reference list in alphabetical order, last name, first initials.

We have included some additional .bst files that may or may not be useful. Please note! We use several citation commands to illustrate the different results and the bibliography in this document cannot be used as an example of any specific reference system. It is YOUR responsibility to determine the reference style of the journal you want to emulate and obtain the necessary .bst files to emulate that style.

3.3 Footnotes

To create footnotes you simply use the `\footnote{text}` command.[1] This works well except when it is used inside any environment that produces (or can produce) a

[1] See, it really does work

box.[2] In that case the manual suggests you use `\footnotemark` inside the environment and just outside the environment use `\foottext{text}` to define the text to accompany the footnote mark. [3] Frankly, I have had some trouble making this option work, particularly in the longtable package and recommend that you avoid footnotes inside any “environment” other than the normal text mode if at all possible.[3] I'm repeating our example of the decimal alignment work-around to illustrate the footnotemark - footnotetext example.

Table 3-1. You shouldn't have two tables (or figures) with the same caption. Even if there's a small difference well into the caption it is best to put the difference first to uniquely identify the table or figure.

Category	Result
first	3.14159[4]
second	16.2
third	123.456

[2] I've seen examples of documents that failed to compile simply because of the placement of a footnote command.

[3] Footnotes should be single-spaced with a space between each note. They should also start re-numbering at one each chapter!

[4] This is an example of the footnotemark process for box creating environments - I sure hope this works!

CHAPTER 4
QUANTUM CHEMISTRY

I've borrowed a few examples of equations I've run across to illustrate how the equations should look in the thesis or dissertation.

4.1 The Electronic Problem

The starting point of any discussion of quantum mechanics is the non-relativistic, time-dependent Shrödinger equation [**?**],

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = \hat{H}\Psi(r,t) \quad , \tag{4–1}$$

where $\hbar$ is Planck's constant, $\Psi(r,t)$ is the wave function of the quantum system and $\hat{H}$ is the Hamiltonian, which is an operator that contains a kinetic energy term and a potential energy term.

When we restrict the wave function to be a product of a function of time and a function of space, as, for example, is the case when the potential energy term of the Hamiltonian is independent of time, the time-independent Scrhödinger equation can be expressed as:

$$\hat{H}\Psi = E\Psi \quad . \tag{4–2}$$

The specific form of the Hamiltonian for molecules is:

$$\begin{aligned}\hat{H} = &-\sum_{A=1}^{M}\frac{1}{2M_A}\nabla_A^2 - \sum_{i=1}^{N}\frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} \\ &+\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}} \quad ,\end{aligned} \tag{4–3}$$

where A and B, etc., label nuclei, and *i*, *j*, etc., label electrons, Z is the atomic number, and Hartree atomic units ($\hbar = e = m_e = 1$) have been used.

The Born-Oppenheimer approximation, which is a useful and central approximation in quantum chemistry, separates electronic and nuclear motions. Assuming that the nuclei are fixed (since nuclei are much heavier than the electrons), the nuclear kinetic energy term, which is the first term in equation (4–3), can be neglected, and the repulsion between nuclei, the third term of equation (4–3), is a constant. This approximation leads to an electronic Hamiltonian,

$$\hat{H}_{elec} = -\sum_{i=1}^{N} \frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}} \quad , \tag{4–4}$$

and the Schrödinger equation becomes:

$$\hat{H}_{elec}\Psi_{elec} = E_{elec}\Psi_{elec} \quad . \tag{4–5}$$

4.2 Hartree-Fock Approximation

Except for the simple case of H_2^+, molecules are many-electron problems and determining accurate molecular orbitals, which are the eigenfunctions of the Schrödinger equation for a molecule, has been the main task of quantum chemists for many years. Approximate methods have been developed to solve the Schrödinger equation, since it is intractable computationally to find the exact solution for a many-electron system. One approximate method that is used frequently to solve the Schrödinger equation is based on Hartree-Fock theory. In the present work, Hartree-Fock is not the main method used, but it is crucial to introduce it to explain the methods on which this work is based.

Consider a trial function in the form of a single N-electron Slater-determinant, which obeys the Pauli exclusion principle,

$$\mid \Psi\rangle = \hat{O}\hat{A} \mid \phi_1\phi_2 ... \phi_\alpha ... \phi_N\rangle \quad . \tag{4–6}$$

Here $\hat{O}$ is the spin projector operator that ensures that the wave function remains an eigenfunction of the spin-squared operator ($\hat{S}^2$), $\hat{A}$ is the antisymmetrizer, ϕ_α is a one-electron wave function that represents the molecular orbital, and Dirac notation has been adopted.

The molecular orbitals can be expanded as a linear combination of atomic orbitals ψ_α ,

$$\phi_i = \sum_u \chi_u C_{ui} = XC_i \quad , \tag{4–7}$$

which constitute the basis set for the calculation.

Ψ is varied with respect to C following the variational principle to minimize the expectation value of the electronic Hamiltonian, $\hat{H}$ (where the electronic subscript has been dropped for simplicity) to give the following expression for the effective one-particle Fock operator, f,

$$f \mid \phi_i\rangle = [h + \sum_{j=1}^{N} J_j - K_j] \mid \phi_i\rangle = \sum_{j=1}^{N} \epsilon_{ji} \mid \phi_j\rangle \quad , \tag{4–8}$$

where h represents the first two terms of equation (4–4) and J and K are the coulomb and exchange operators respectively. Using a unitary basis to diagonalize the Hermitian matrix, ϵ, with matrix elements ϵ_{ji} yields the canonical Hartree-Fock equation,

$$f\phi_i = \epsilon_i\phi_i \quad . \tag{4–9}$$

From this equation the following generalized-eigenvalue expression can be obtained,

$$FC = SCE \quad , \tag{4–10}$$

where F is the Fock matrix, C is a square matrix containing the molecular orbital coefficients, S is the overlap matrix and E is the energy matrix containing the orbital energies ϵ_i.

The Fock matrix elements are,

$$\begin{aligned} F_{uv} &= \langle \chi_u \mid f \mid \chi_v \rangle = \langle u \mid f \mid v \rangle \\ &= H_{uv} + \sum_{s,t} P_{st}[\langle us \mid vt \rangle - \frac{\langle us \mid tv \rangle}{2}] \quad , \end{aligned} \tag{4–11}$$

P is the density matrix,

$$P_{uv} = \sum_{a} C_{ua} C_{va} n_a \quad , \tag{4–12}$$

where n_a is the occupation number.

The overlap matrix elements are,

$$S_{uv} = \langle \chi_u \mid \chi_v \rangle = \langle u \mid v \rangle \quad . \tag{4–13}$$

A self-consistent solution of the previous equations is known as the Hartree-Fock, Self-Consistent Field (SCF) methodology.

These *ab initio* expressions for the Fock matrix will be used below to explain additional details of the methods used in this research.

CHAPTER 5
MATH, FIGURES, AND TABLES

5.1 Text Flow: Problems and Solutions

Let's face it. LaTeX is used because you can type very complicated formulas and equations without ever touching a mouse! And in most situations, where the spacing requirements are not as demanding as the UF Theses and Dissertation requirements, LaTeX's love of white space would not pose a problem.

However, you ARE producing this document for the UF Graduate School and their spacing requirements ARE quite demanding. Pages, other than the last page of a chapter, are supposed to be full. LaTeX has a tendency to break a page early rather than split a display element (equation array, align, theorem, table, figure, etc.). To help in this matter there are three lines in the preamble of the ufsampleETD.tex file. These are:

```
\renewcommand{\topfraction}{0.85}
\renewcommand{\textfraction}{0.1}
\renewcommand{\floatpagefraction}{0.75}
```

However, even with these commands LaTeX likes to break pages rather than equation arrays, theorems, postulates, proofs, etc. If you find that these elements are causing pages to break badly you can un-comment the command `\allowdisplaybreaks` and with any luck, that will cure the problem. If not, it may be necessary to break the displays manually which is always the last resort and only done just before final submission.

5.2 Equation Notes

Again, one of the major reasons for using LaTeX in the first place is how it handles the mathematics displays. However, there are a few details you need to be aware of:

- If you place an extra carriage return before or after an equation LaTeX will place some extra "paragraph" spacing around the equation. Try to avoid this.
- If you want to explain your notation in the equation with a list of statements such as; where $Z = \gamma$, do so in paragraph form rather than a vertical list.

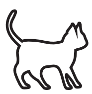
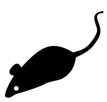
- Every equation does not have to be labeled. Only those you will refer to in the text. If it is simply part of the paragraph it can be displayed as an equation but doesn't have to be labeled. Just remember the `\noindent` command to continue the text after the display.

5.3 Tables, Figures, and Subfigures

5.3.1 Tables

Typically, the standard LaTeX table environment is used. Table captions need to be above the table, and typically there should not be any vertical lines in the table. Formatting tables in a landscape page is explained in section 5.4.

Table 5-1. A sample Table

First	Second
12	26
17	93
text	can be there too.
	Figures too - a cat.
	and a mouse!

5.3.2 Figures

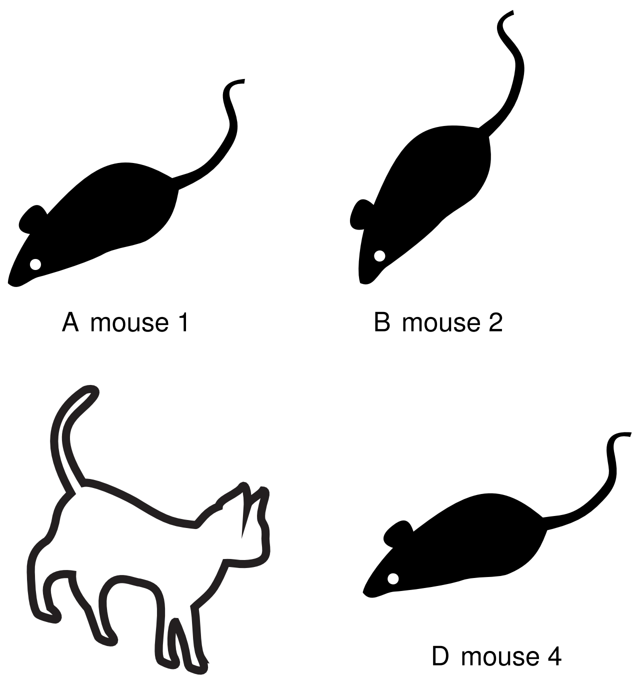
You can either use `\includegraphics` or \epsfig commands to include your figures. The appropriate packages are included in the packages.tex file. For additional precaution, a copy of `rotating.sty` is included in the template. Please do not delete this file. Note that the caption for the figures is below the figure. The figures in the table above was inserted with \epsfig. Below is a sample file with `\includegraphics`:

Figure 5-1. LaTeX2ϵ logo, resized for no reason. This caption is being extended in order to test that it has the correct indentation.

5.3.3 Subfigures

In addition to the standard LaTeX options for scaling and rotation, the `rotating` package has additional options for turning and rotating both text and figures/tables. Please look at the documentation of this package for further details.

For subfigures, please use `subfigure` command (see `chapter4.tex` for code). We have made some slight modifications to the subfigure.sty file to match the Editorial Office specification so make sure it is in the same folder as the ufsampleETD.tex file when you compile your document.



A mouse 1

B mouse 2

C Hungry Cat

D mouse 4

Figure 5-2. Tom and Jerries?

There is some fancy formatting possible with `subfigure`. For instance, it is possible (but not suggested) to list the captions of each subfigure in the List of Figures in the table of contents. Please look at the documentation of `subfigure` package for details.

5.4 Formatting in Landscape Mode

There are many ways to format figures and tables in a landscape. Depending on what you want to use, you can use one of the following enviroments:

- The `landscape` environment
- The `sidewaysfigure` environment
- The `sidewaystable` environment

5.4.1 The `landscape` environment

The `landscape` environment starts by default a new page, because it changes the two lengths \paperwidth and \paperheight. Typically you will use the `landscape` if you want to have an **entire** section or a subsection in landscape mode (i.e. both text and figures/tables). This should not be used for a just single figure or a table (Use `sidewaysfigure` and `sidewaystable` described in sub-section 5.4.2 instead). In the chapter4.tex file we demonstrate how to force a page break in the Table of Contents. Something that often needs to be done but is not documented in most LaTeX tutorials.

The following sub-subsection is included in an environment like:

```
\begin{landscape}
\subsubsection{Sample Landscape Page}\label{ps}
Note that even though we are in landscape mode,
only the text part is in landscape.
The header and footer (for example the page number) are still
in portrait mode. This $\backslash$begin$\{$landscape$\}$
environment is part of the lscape package. Look at the documentation
of this package for further details and options.
\end{landscape}
```

The \begin{landscape} immediately starts the new page, a lot of vertical whitespace, like the one on this page, maybe possible.

The subsubsection command also represents a common error in dissertation/thesis construction. There is only one heading at that level. Whenever a section is divided, it must be divided into two segments - otherwise there is no reason to introduce another category.

5.4.1.1 Sample Landscape Page

Note that even though we are in landscape mode, only the text part is in landscape, the header and footer (that implement, for example the page number) are still in portrait mode. This `landscape` environment is part of the `lscape` package. Look at the documentation of this package for more details and options.

5.4.2 `sidewaysfigure` and `sidewaystable` Environments

With large figures and tables with lots of columns, it is sometimes necessary to rotate them to landscape mode. The `sidewaysfigure` and the `sidewaystable` environments from the `rotating` package can be used for this. Sample code for these two environments are give below:

A Landscape Figure:

```
\begin{sidewaysfigure}
\centerline{\epsfig{figure=figurename.eps, scale=0.5}}
\caption{Your Caption for the figue}
\end{sidewaysfigure}

Note: Change value of scale to change your figure size.
      1 is 100%, i.e. original size. You can go beyond 1
      if your file is in a scalable vector graphics format
      like .eps
```

A Landscape Table:

```
\begin{sidewaystable}
\centering %optional
\begin{tabular}{rl}
\end{tabular}
\caption{Your Caption for the table}
\end{sidewaystable}
```

The above code will produce a figure/table rotated by 90° in the counter-clockwise direction, and will also rotate the caption accordingly as per the Editorial Office requirements. Both these environments are “intelligent” in the sense that they will put your figure/table in a new landscape page and will **NOT** leave empty whitespace before the figure like the `landscape` environment. The following ’Lorem Ipsum’ paragraphs demonstrate this.

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Integer ante. Ut tincidunt ultrices turpis. Phasellus nonummy pulvinar sem. Donec sem nisl, rhoncus eu, porttitor in, blandit nec, arcu. Vestibulum tincidunt ante. Pellentesque quis massa. Proin vehicula feugiat turpis. Aenean at tellus sed justo ornare dictum. Nullam sit amet libero nec lorem sodales cursus. Donec tortor nulla, convallis in, suscipit in, posuere at, nunc.

Figure 5-3. You can turn the world on its heels.

Aliquam tortor risus, ultricies sed, eleifend in, congue quis, justo. Pellentesque egestas orci non urna. Phasellus ligula. Ut nonummy. Suspendisse potenti. Donec posuere justo quis eros. In erat. Nunc aliquam metus sed dui. Fusce justo felis, posuere a, elementum non, semper eget, mi. Morbi iaculis lorem at sem. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Phasellus velit. Maecenas libero tortor, pharetra id, dictum ac, lacinia vestibulum, urna. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. In libero nunc, fringilla a, condimentum lobortis, consequat eget, quam. Phasellus eget nisi. Maecenas risus ligula, euismod a, tristique non, sagittis eu, quam. Donec metus nunc, varius ut, lacinia sit amet, pellentesque ac, mauris. Nulla mollis aliquam metus.

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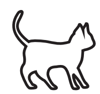
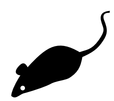
Aliquam tortor risus, ultricies sed, eleifend in, congue quis, justo. Pellentesque egestas orci non urna. Phasellus ligula. Ut nonummy. Suspendisse potenti. Donec posuere justo quis eros. In erat. Nunc aliquam metus sed dui. Fusce justo felis, posuere a, elementum non, semper eget, mi. Morbi iaculis lorem at sem. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Phasellus velit. Maecenas libero tortor, pharetra id, dictum ac, lacinia vestibulum, urna. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. In libero nunc, fringilla a, condimentum lobortis, consequat eget, quam. Phasellus eget nisi. Maecenas risus ligula, euismod a, tristique non, sagittis eu, quam. Donec metus nunc, varius ut, lacinia sit amet, pellentesque ac, mauris. Nulla mollis aliquam metus.

Table 5-2. The Same Table as C.1, but in landscape mode

First	Second
12	26
17	93
text	can be there too.
	Figures too - a cat.
	and a mouse!

5.5 Some bugs and fixes

A quirk in the $\LaTeX2\epsilon$ template is the centering of table and figure captions . . . which the editorial office will not accept. This is actually only a problem for captions that are less than the width of the paper(within the margins that is). A fix has already been implemented in the template for this issue.

However, if you find your short captions are being centered in spite of the new caption package options, try using the following codes, which each differ ever so slightly depending if the caption is for a table or figure. Inserting the given code in the table or figure environments just after you declare the start of that environment for each table or \landscape environment figure that has a short caption that is being centered:

For Tables:

```
  \makeatletter
\long\def\@makecaption#1#2{%
  \vskip\abovecaptionskip
  \sbox\@tempboxa{#1: #2}%
  \ifdim \wd\@tempboxa >\hsize
    #1: #2\par
  \else
    \global \@minipagefalse
    \hb@xt@\hsize{\box\@tempboxa\hfil}%
  \fi}
\makeatother
```

For Figures:

```
\makeatletter
\long\def\@makecaption#1#2{%
  \vskip\abovecaptionskip
  \sbox\@tempboxa{#1: #2}%
  \ifdim \wd\@tempboxa >\hsize
    #1: #2\par
  \else
    \global \@minipagefalse
    \hb@xt@\hsize{\box\@tempboxa\hfil}%
  \fi
  \vskip\belowcaptionskip}
\makeatother
```

CHAPTER 6
GENERAL THESIS TIPS

- BACK UP YOUR THESIS. Often you will not realize for days or weeks that important paragraph or page is missing. Make recovery as easy as possible by keeping a dated backup of each writing session. Then copy those backups to at least two locations other than your hard drive: your home server, gmail account, thumb drive, the options are wide and numerous. There is no excuse for not backing up the most important document of your academic career.

- Start your bibliographic database the day you start reading. Keep it up to date and annotate it, so you know where it came from (library, Internet, public library, professor), whether you've read it, and where you want to cite it. This will make the writing process less frustrating and creating the bibliography seamless.

- Think of thesis formatting as a form of productive procrastination. Please don't put it off until the last week.

- BACK UP. No, seriously. It's not "if" your hard drive fails, it's "when." Not to scare you or anything, but it's a good habit, like buckling your seat belt or not leaving your laptop unattended. You really don't want to wish you had taken that small precaution.

- Keep the editable original of each graphic you want to include in your thesis in one folder. Later you may need to change a graphic quickly and having the editable original makes it easy. For graphs, keep the original Excel/JMP/Stata document, not a PDF. For photographs, keep a high resolution copy. For drawings and illustrations, keep the original document.

- Use the timesaving benefits of LaTeX from the first day. Cross references can refer to tables, graphics, and chapters so you do not have to update references as your thesis changes. Use comments to make notes about what needs to added or changed.

- Enjoy the experience! And get some sleep, food and relaxation on occasion. Thousands of people did this before you; you can do this too.

APPENDIX A
THIS IS THE FIRST APPENDIX

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Maecenas eget magna. Aenean et lorem. Ut dignissim neque at nisi. In hac habitasse platea dictumst. In porta ornare eros. Nunc eu ante. In non est vehicula tellus cursus suscipit. Proin sed libero. Sed risus enim, eleifend in, pellentesque ac, nonummy quis, nulla. Phasellus imperdiet libero nec massa. Ut sapien libero, adipiscing eu, volutpat porttitor, ultricies eget, nisi. Sed odio. Suspendisse potenti. Duis dolor augue, viverra id, porta in, dignissim id, nisl. Vivamus blandit cursus eros. Maecenas sit amet urna sit amet orci nonummy pharetra.

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APPENDIX B
AN EXAMPLE OF A HALF TITLE PAGE

$\LaTeX\,2_{\varepsilon}$

Figure B-1. $\LaTeX 2_\epsilon$. logo

This is how a section should look if the first page is a landscape page. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut sit amet nulla. Integer mauris turpis, dapibus ac, auctor non, vehicula sit amet, magna. Suspendisse eu tellus. Etiam porta. Donec magna. Donec ut dui. In hac habitasse platea dictumst. Nullam suscipit, mi at adipiscing commodo, lorem erat scelerisque erat, non pulvinar leo mi eu metus. Phasellus id felis. Sed quam purus, molestie quis, ultrices nec, dictum at, magna. Proin viverra viverra ante.

Maecenas sagittis magna quis ligula. Duis vestibulum mi a felis. Aenean accumsan mattis massa. Nullam lacus sem, consectetuer non, condimentum sit amet, pharetra ac, odio. Morbi nisi magna, tincidunt sed, placerat nec, tincidunt id, lectus. Donec ac dui non mauris vulputate aliquam. Nullam scelerisque congue pede. Integer ipsum. Vestibulum auctor. Suspendisse eget leo id libero cursus dictum. Sed malesuada. Aliquam imperdiet. Donec dui metus, porta eu, aliquet vel, vulputate vitae, lacus.

Nulla quis purus id turpis luctus feugiat. Fusce feugiat. Proin felis. Morbi elit est, fermentum in, tincidunt vitae, convallis vel, orci. Vestibulum justo. Suspendisse non nisl. Pellentesque pretium adipiscing elit. Phasellus fermentum consequat augue. Sed pede nisl, fermentum vel, vulputate id, sollicitudin sed, ligula. Cras suscipit, quam et euismod sagittis, nisl felis gravida felis, quis pulvinar purus est vel pede. Suspendisse mattis est ac nunc. Curabitur rutrum, turpis sit amet commodo tempus, metus lorem commodo lectus, eget fringilla justo nisi et purus. Ut quam sapien, vehicula quis, rhoncus non, sagittis nec, risus.

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Phasellus vitae dui id orci sodales cursus. Curabitur sed nulla quis mauris tincidunt iaculis. Vivamus semper semper orci. Phasellus suscipit ante vitae leo. Sed arcu ipsum, condimentum id, luctus in, sodales eu, magna. In dictum, arcu quis pharetra vestibulum, ante enim placerat lacus, vitae placerat est leo vitae elit. Pellentesque bibendum enim vulputate eros. Nunc laoreet. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Praesent purus odio, euismod sit amet, aliquam a, volutpat in, augue. Phasellus id massa. Suspendisse suscipit ligula pharetra dolor. Pellentesque vel pede.

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APPENDIX C
DERIVATION OF THE Υ FUNCTION

Proposition C.1. *The Upsilon Function*

(1) If $\beta > 0$ and $\alpha \neq 0$, then for all $n \geq -1$,

$$I_n(c;\alpha;\beta;\delta) = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i}Hh_i(\beta c - \delta)$$

$$+(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c + \delta + \frac{\alpha}{\beta})$$

(2) If $\beta < 0$ and $\alpha < 0$, then for all $x \geq -1$

$$I_n(c;\alpha;\beta;\delta) = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i}Hh_i(\beta c - \delta)$$

$$-(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(\beta c - \delta - \frac{\alpha}{\beta})$$

Proof. Case 1. $\beta > 0$ and $\alpha \neq 0$. Since, for any constant α and $n \geq 0$, $e^{\alpha x}Hh_n(\beta x - \delta) \to 0$ as $x \to \infty$ thanks to (B4), integration by parts leads to

$$I_n = -\frac{1}{\alpha}Hh(\beta c - \delta)e^{\alpha c} + \frac{\beta}{\alpha}\int_c^{\infty} e^{\alpha x}Hh_{n-1}(\beta c - \delta)dx$$

In other words, we have a recursion, for $n \geq 0$, $I_n = -(e^{\alpha c}\alpha)Hh_n(\beta c - \delta) + (\frac{\beta}{\alpha})I_{n-1}$ with

$$I_{-1} = \sqrt{2\pi}\int_c \infty e^{\alpha x}\varphi(-\beta x + \delta)dx$$

$$= \frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c + \delta + \frac{\alpha}{\beta})$$

Solving it yields, for $n \geq -1$,

$$I_n = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{i}Hh_{n-i}(\beta c + \delta) + (\frac{\beta}{\alpha})^{n+1}I_{-1}$$

$$= -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i}Hh_i(\beta c+\delta)$$

$$+(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c+\delta+\frac{\alpha}{\beta})$$

where the sum over an empty set is defined to be zero. □

Case2. $\beta < 0$ *and* $\alpha < 0$*. In this case, we must also have, for* $n \geq 0$ *and any constant* $\alpha < 0$, $e^{\alpha x}Hh_n(\beta x-\delta) \to 0$ *as* $x \to \infty$*, thanks to (B5). Using integration by parts, we again have the same recursion, for* $n \geq 0$, $I_n = -(e^{\alpha c}/\alpha)Hh_n(\beta c-\delta)+(\beta/\alpha)I_{n-1}$*, but with a different initial condition*

$$I_{-1} = \sqrt{2\pi}\int_c^{\infty} e^{\alpha x}\varphi(-\beta x+\delta)dx$$

$$= -\frac{\sqrt{2\pi}}{\beta}exp\{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}\}\phi(\beta c-\delta-\frac{\alpha}{\beta})$$

Solving it yields (B8), for $n \geq -1$*.*

Finally, we sum the double exponential and the normal random variables

Proposition B.3.

Suppose $\{\xi_1, \xi_2, ...\}$ *is a sequence of i.i.d. exponential random variables with rate* $\eta > 0$*, and Z is a normal variable with distribution* $N(0, \sigma^2)$*. Then for every* $n \geq 1$*, we have: (1) The density functions are given by:*

$$f_{Z+\sum_{i=1}^n \xi_i}(t) = (\sigma\eta)^n\frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}}e^{-t\eta}Hh_{n-1}(-\frac{t}{\sigma}+\sigma\eta)$$

$$f_{Z-\sum_{i=1}^n \xi_i}(t) = (\sigma\eta)^n\frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}}e^{-t\eta}Hh_{n-1}(\frac{t}{\sigma}+\sigma\eta)$$

(2) The tail probabilities are given by

$$P(Z+\sum_{i=1}^{n}\xi_i \geq x) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} I_{n-1}(x; -\eta, -\frac{1}{\sigma}, -\sigma\eta)$$

$$P(Z-\sum_{i=1}^{n}\xi_i \geq x) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} I_{n-1}(x; \eta, \frac{1}{\sigma}, -\sigma\eta)$$

Proof. Case 1. The densities of $Z+\sum_{i=1}^{n}\xi_i$, *and* $Z-\sum_{i=1}^{n}\xi_i$. *We have*

$$f_{Z+\sum_{i=1}^{n}\xi_i}(t) = \int_{-\infty}^{\infty} f_{\sum_{i=1}^{n}\xi_i}(t-x) f_Z(x) dx$$

$$= e^{-t\eta}(\eta^n) \int_{-\infty} t \frac{e^{x\eta}(t-x)^{n-1}}{(n-1)!} \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/(2\sigma^2)} dx$$

$$= e^{-t\eta}(\eta^n) e^{(\sigma\eta)^2/(2)} \int_{-\infty} t \frac{(t-x)^{n-1}}{(n-1)!} \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\sigma^2\eta)^2/(2\sigma^2)} dx$$

Letting $y = (x-\sigma^2\eta)/\sigma$ *yields*

$$f_{Z+\sum_{i=1}^{n}\xi_i}(t) = e^{-t\eta}(\eta^n) e^{(\sigma\eta)^2/(2)} \sigma^{n-1}$$

$$\times \int_{-\infty}^{t/\sigma-\sigma\eta} \frac{(t/\sigma - y - \sigma\eta)^{n-1}}{(n-1)!} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy$$

$$= \frac{e^{(\sigma\eta)^2/2}}{\sqrt{2\pi}} (\sigma^{n-1}\eta^n) e^{-t\eta} Hh_{n-1}(-t/\sigma + \sigma\eta)$$

because $(1/(n-1)!) \int_{-\infty} a(a-y)^{n-1} e^{-y^2/2} dy = Hh_{n-1}(a)$. *The derivation of* $f_{Z+\sum_{i=1}^{n}\xi_i}(t)$ *is similar.*

Case 2. $P(Z+\sum_{i=1}^{n}\xi_i \geq x)$ *and* $P(Z-\sum_{i=1}^{n}\xi_i \geq x)$. *From (B9), it is clear that*

$$P(Z+\sum_{i=1}^{n}\xi_i \geq x) = \frac{(\sigma\eta)^n e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} \int_{x}^{\infty} e^{(-i\eta)} Hh_{n-1}(-\frac{t}{\sigma} + \sigma\eta) dt$$

$$= \frac{(\sigma\eta)^n e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} I_{n-1}(x; -\eta, -\frac{1}{\sigma}, -\sigma\eta) dt$$

by (B6). We can compute $P(Z - \sum_{i=1}^n \xi_i \geq x)$ *similarly.*

Theorem C.1. *Theorem With* $\pi_n := P(N(t) = n) = e^{-\lambda T}(\lambda T)^n/n!$ *and* I_n *in Proposition C.1. , we have*

$$P(Z(T) \geq a) = \frac{e^{(\sigma\eta_1)^2 T/2}}{\sigma\sqrt{2\pi T}} \sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} P_{n,k}(\sigma\sqrt{T}\eta_1)^k \times I_{k-1}(a - \mu T; -\eta_1, -\frac{1}{\sigma\sqrt{T}}, -\sigma\eta_1\sqrt{T})$$

$$+\frac{e^{(\sigma\eta_2)^2 T/2}}{\sigma\sqrt{2\pi T}} \sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} Q_{n,k}(\sigma\sqrt{T}\eta_2)^k$$

$$\times I_{k-1}(a - \mu T; \eta_2, \frac{1}{\sigma\sqrt{T}}, -\sigma\eta_2\sqrt{T})$$

$$+\pi_0\phi(-\frac{a - \mu T}{\sigma\sqrt{T}})$$

Proof by the decomposition (B2)

$$P(Z(T) \geq a) = \sum_{n=0}^{\infty} \pi_n P(\mu T + \sigma\sqrt{T}Z + \sum_{j=1}^{n} Y_j \geq a)$$

$$= \pi_0 P(\mu T + \sigma\sqrt{T}Z \geq a)$$

$$+\sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} P_{n,k} P(\mu T + \sigma\sqrt{T}Z + \sum_{j=1}^{n} \xi_j^+ \geq a)$$

$$+\sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} Q_{n,k} P(\mu T + \sigma\sqrt{T}Z - \sum_{j=1}^{n} \xi_j^- \geq a)$$

The result now follows via (B11) and (B12) for $\eta_1 > 1$ *and* $\eta_2 > 0$.

APPENDIX D
DERIVATION OF THE Υ FUNCTION

Proposition B.3.

Suppose $\{\xi_1, \xi_2, ...\}$ is a sequence of i.i.d. exponential random variables with rate $\eta > 0$, and Z is a normal variable with distribution $N(0, \sigma^2)$. Then for every $n \geq 1$, we have: (1) The density functions are given by:

$$f_{Z+\sum_{i=1}^n \xi_i}(t) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} Hh_{n-1}(-\frac{t}{\sigma} + \sigma\eta)$$

$$f_{Z-\sum_{i=1}^n \xi_i}(t) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} Hh_{n-1}(\frac{t}{\sigma} + \sigma\eta)$$

(2) The tail probabilities are given by

$$P(Z + \sum_{i=1}^n \xi_i \geq x) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} I_{n-1}(x; -\eta, -\frac{1}{\sigma}, -\sigma\eta)$$

$$P(Z - \sum_{i=1}^n \xi_i \geq x) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} I_{n-1}(x; \eta, \frac{1}{\sigma}, -\sigma\eta)$$

Proof. Case 1. The densities of $Z + \sum_{i=1}^n \xi_i$, and $Z - \sum_{i=1}^n \xi_i$. We have

$$f_{Z+\sum_{i=1}^n \xi_i}(t) = \int_{-\infty}^{\infty} f_{\sum_{i=1}^n \xi_i}(t-x) f_Z(x) dx$$

$$= e^{-t\eta}(\eta^n) \int_{-\infty} t \frac{e^{x\eta}(t-x)^{n-1}}{(n-1)!} \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/(2\sigma^2)} dx$$

$$= e^{-t\eta}(\eta^n) e^{(\sigma\eta)^2/(2)} \int_{-\infty} t \frac{(t-x)^{n-1}}{(n-1)!} \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\sigma^2\eta)^2/(2\sigma^2)} dx$$

Letting $y = (x - \sigma^2\eta)/\sigma$ yields

$$f_{Z+\sum_{i=1}^n \xi_i}(t) = e^{-t\eta}(\eta^n) e^{(\sigma\eta)^2/(2)} \sigma^{n-1}$$

$$\times \int_{-\infty}^{t/\sigma-\sigma\eta} \frac{(t/\sigma - y - \sigma\eta)^{n-1}}{(n-1)!} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy$$

$$= \frac{e^{(\sigma\eta)^2/2}}{\sqrt{2\pi}} (\sigma^{n-1}\eta^n) e^{-t\eta} Hh_{n-1}(-t/\sigma + \sigma\eta)$$

because $(1/(n-1)!) \int_{-\infty} a(a-y)^{n-1} e^{-y^2/2} dy = Hh_{n-1}(a)$. The derivation of $f_{Z+\sum_{i=1}^n \xi_i}(t)$ is similar.

Case 2. $P(Z + \sum_{i=1}^n \xi_i \geq x)$ and $P(Z - \sum_{i=1}^n \xi_i \geq x)$. From (B9), it is clear that

$$P(Z + \sum_{i=1}^n \xi_i \geq x) = \frac{(\sigma\eta)^n e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} \int_x^{\infty} e^{(-i\eta)} Hh_{n-1}(-\frac{t}{\sigma} + \sigma\eta) dt$$

$$= \frac{(\sigma\eta)^n e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} I_{n-1}(x; -\eta, -\frac{1}{\sigma}, -\sigma\eta) dt$$

by (B6). We can compute $P(Z - \sum_{i=1}^n \xi_i \geq x)$ similarly.

Theorem B.1. With $\pi_n := P(N(t) = n) = e^{-\lambda T}(\lambda T)^n/n!$ and I_n in Proposition B. , we have

$$P(Z(T) \geq a) = \frac{e^{(\sigma\eta_1)^2 T/2}}{\sigma\sqrt{2\pi T}} \sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} P_{n,k}(\sigma\sqrt{T}\eta_1)^k \times I_{k-1}(a - \mu T; -\eta_1, -\frac{1}{\sigma\sqrt{T}}, -\sigma\eta_1\sqrt{T})$$

$$+\frac{e^{(\sigma\eta_2)^2 T/2}}{\sigma\sqrt{2\pi T}} \sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} Q_{n,k}(\sigma\sqrt{T}\eta_2)^k$$

$$\times I_{k-1}(a - \mu T; \eta_2, \frac{1}{\sigma\sqrt{T}}, -\sigma\eta_2\sqrt{T})$$

$$+\pi_0 \phi(-\frac{a - \mu T}{\sigma\sqrt{T}})$$

Proof by the decomposition (B2)

APPENDIX E
THIS IS THE FIRST APPENDIX

Proof of Proposition 1.

(1) Since B(T,T)=1, Equation (8) yields

$$B(t,T) = e^{\theta(T-t)} \frac{E((\delta(T))^{\alpha-1}|\mathfrak{F}_t)}{(\delta(t))^{\alpha-1}}$$

Using the fact that

$$(\frac{\delta(T)}{\delta(t)})^{\alpha-1} = exp(\alpha-1)(\mu_1 - \frac{1}{2}\sigma_1^2)(T-t) + \sigma_1(\alpha-1)(W_1(T)-W_1(t)) \prod_{i=N(t)+1}^{N(T)} \widetilde{V}_i^{\alpha-1}$$

$$E(\prod_{i=N(t)+1}^{N(t)} \widetilde{V}_i^{\alpha-1}) = \sum_{j=0} \infty e^{-\lambda(T-t)} \frac{[\lambda(T-t)]^j}{j!} \zeta_1^{(\alpha-1)} + 1^j$$
$$= exp\lambda\zeta_1^{(\alpha-1)}(T-t)$$

First equation yields

$$B(t,T) = exp[-(T-t)\theta - (\alpha-1)(\mu_1 - \frac{1}{2}\sigma_1^2) - \frac{1}{2}\sigma_1^2(\alpha-1)^2 - \lambda\zeta_1^{(\alpha-1)}]$$

Note that it implies

$$e^{-r(T-t)} = E(U_c(\delta(T),T)/U_c(\delta(t),t)|\mathfrak{F}_t)$$

which shows that Z(t) is a martingale under P. Furthermore, it leads to

$$Z(t) = (\delta(0))^{\alpha-1} e^{(r-\theta)t} exp(\alpha-1)(\mu_1 - \frac{1}{2}\sigma_1^2)t + \sigma_1(\alpha-1)(W_1(t)) \prod_{i=1}^{N(t)} \widetilde{V}_i^{\alpha-1}$$

$$= (\delta(0))^{\alpha-1} exp - \frac{1}{2}\sigma_1^2(\alpha-1)^2 - \lambda\zeta_1^{(\alpha-1)} t + \sigma_1(\alpha-1)(W_1(t)) \prod_{i=1}^{N(t)} \widetilde{V}_i^{\alpha-1}$$

Now

$$\psi_s(t) = \frac{E(U_c(\delta(T),T)\psi_s(T)|\mathfrak{F}_t)}{(U_c(\delta(t),t))} = e^{-rT}E\{\frac{Z(T)}{Z(t)}\psi_s(T)|\mathfrak{F}_t\}$$
$$= e^{-rT}E^*(\psi_s(T)|\mathfrak{F}_t)$$

Proof of Theorem 1. The Girsanov theorem for jump-diffusion processes tells us that under P^*, $W_1'(t) = W_1(t) - \sigma_1(\alpha-1)t$ is a new Brownian motion and under P^* the jump rate of N(t) is $\lambda^* = \lambda E(\widetilde{V}_i^{\alpha-1}) = \lambda(\zeta_1^{(\alpha-1)}+1)$ and $\widetilde{V}_i$ has a new density $f^*_{\widetilde{V}}(x) = (1/(\zeta_1^{(\alpha-1)}+1))x^{\alpha-1}f_{\widetilde{V}}(x)$. Therefore, dynamics of S(t) is given by

$$\frac{dS(t)}{S(t-)} = \mu dt + \sigma\{\rho dW_1(t) + \sqrt{1-\rho^2}dW_2(t)\} + \Delta(\sum_{i=1}^{N(t)}(V_i^\beta - 1))$$

$$= \{\mu + \sigma_1\sigma\rho(\alpha-1)dt + \sigma\{\rho dW_1'(t) + \sqrt{1-\rho^2}dW_2(t)\} + \Delta(\sum_{i=1}^{N(t)}(V_i^\beta - 1))$$

Because

$$E^*(\widetilde{V}_i^\beta) = \int_0^\infty x^\beta \frac{1}{\zeta_1^{(\alpha-1)}+1}x^{(\alpha-1)}f_{\widetilde{V}}(x)dx$$
$$= \frac{1}{\zeta_1^{(\alpha-1)}+1}E(\widetilde{V}^{\alpha+\beta-1}) = \frac{\zeta_1^{\alpha+\beta-1}+1}{\zeta_1^{\alpha-1}+1}$$

we have

$$\lambda^*\{E^*(\widetilde{V}^\beta) - 1\} = \lambda(\zeta_1^{\alpha+\beta-1} - \zeta_1^{\alpha-1})$$

.

Therefore

$$\frac{dS(t)}{S(t-)} = \{\mu + \sigma_1\sigma\rho(\alpha-1) + \lambda(\zeta_{\alpha+\beta-1} - \zeta_{\alpha-1})\}dt$$

$$-\lambda^*\{E^*(\widetilde{V}^\beta) - 1\}dt + \sigma\{\rho dW_1'(t) + \sqrt{1-\rho^2}dW_2(t)\} + \Delta(\sum_{i=1}^{N(t)}(V_i^\beta - 1))$$

Hence to satisfy the rational equilibrium requirement $S(t) = e^{-r(T-t)}E^*(S(T)|\mathfrak{F})$ we must have $\mu + \sigma_1\sigma\rho(\alpha - 1) + \lambda(\zeta_{\alpha+\beta-1} - \zeta_{\alpha-1}) = r$

So, under the measure P^*, the dynamics of S(t) is given by

$$\frac{dS(t)}{S(t-)} = rdt - \lambda^*\{E^*(\widetilde{V}^\beta) - 1\}dt + \sigma\{\rho dW_1'(t) + \sqrt{1-\rho^2}dW_2(t)\} + \Delta(\sum_{i=1}^{N(t)}(V_i^\beta - 1))$$

APPENDIX F
DERIVATION OF THE Υ FUNCTION

We first decompose the sum of the double exponential random variables.

The memoryless property of exponential random variables yields $(\xi^+ - \xi^- | \xi^+ > \xi^-) =^d \xi^+$ and $(\xi^+ - \xi^- | \xi^+ < \xi^-) =^d -\xi^-$, thus leading to the conclusion that

$$\xi^+ - \xi^- = \left\{ \begin{array}{cl} \xi^+ & \text{with probability } \eta_2/(\eta_1+\eta_2) \\ -\xi^- & \text{with probability } \eta_1/(\eta_1+\eta_2) \end{array} \right\}.$$

because the probabilities of the events $\xi^+ > \xi^-$ and $\xi^+ < \xi^-$ are $\eta_2/(\eta_1+\eta_2)$ and $\eta_1/(\eta_1+\eta_2)$, respectively. The following proposition extends (B.1.)

Proposition B.1. For every $n \geq 1$, we have the following decomposition

$$\sum_{i=1}^{n} Y_i =^d \left\{ \begin{array}{cl} \sum_{i=1}^{k} \xi_i^+ & \text{with probability } P_{n,k},\ k = 1, 2, ..., n \\ -\sum_{i=1}^{k} \xi_i^- & \text{with probability } Q_{n,k},\ k = 1, 2, ..., n \end{array} \right\}.$$

where $P_{n,k}$ and $Q_{n,k}$ are given by

$$P_{n,k} = \sum_{i=k}^{n-1} \binom{n-k-1}{i-k} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{i-k} (\frac{\eta_2}{\eta_1+\eta_2})^{n-i} p^i q^{n-i}$$

$$1 \leq k \leq n-1$$

$$Q_{n,k} = \sum_{i=k}^{n-1} \binom{n-k-1}{i-k} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{n-i} (\frac{\eta_2}{\eta_1+\eta_2})^{i-k} p^{n-i} q^i$$

$$1 \leq k \leq n-1,\ P_{n,n} = p^n,\ Q_{n,n} = q^n$$

and $\binom{0}{0}$ is defined to be one. Hence ξ_i^+ and ξ_i^- are i.i.d. exponential random variables with rates η_1 and η_2, respectively.

As a key step in deriving closed-form solutions for call and put options, this proposition indicates that the sum of the i.i.d. double exponential random variable can be written, in distribution, as a randomly mixed gamma random variable. To prove Proposition B.1, the following lemma is needed.

Lemma B.1.

$$\sum_{i=1}^{n} \xi_i^+ - \sum_{i=1}^{n} \xi_i^-$$

$$=^d \left\{ \begin{array}{ll} \sum_{i=1}^{k} \xi_i & \text{with probability } \binom{n-k+m-1}{m-1}(\frac{\eta_1}{\eta_1+\eta_2})^{n-k}(\frac{\eta_2}{\eta_1+\eta_2})^{m}, k=1,...,n \\ -\sum_{i=1}^{l} \xi_i & \text{with probability } \binom{n-l+m-1}{n-1}(\frac{\eta_1}{\eta_1+\eta_2})^{n}(\frac{\eta_2}{\eta_1+\eta_2})^{m-l}, l=1,...,m \end{array} \right\}.$$

We prove it by introducing the random variables $A(n, m) = \sum_{i=1}^{n} \xi_i - sum_{j=1}^{m} \tilde{\xi}_j$ Then

$$A(n, m) =^d \left\{ \begin{array}{ll} A(n-1, m-1) + \xi^+ & \text{with probability } \eta_2/(\eta_1+\eta_2) \\ A(n-1, m-1) - \xi^- & \text{with probability } \eta_1/(\eta_1+\eta_2) \end{array} \right\}.$$

$$=^d \left\{ \begin{array}{ll} A(n, m-1) & \text{with probability } \eta_2/(\eta_1+\eta_2) \\ A(n-1, m) & \text{with probability } \eta_1/(\eta_1+\eta_2) \end{array} \right\}.$$

via B.1.. Now suppose horizontal axis that are representing the number of $\{\zeta_i^+\}$ and vertical axis representing the number of $\{\zeta_i^-\}$. Suppose we have a random walk on the integer lattice points. Starting from any point (n, m), $n, m \geq 1$, the random walk goes either one step to the left with probability $\eta_1/(\eta_1+\eta_2)$ or one step down with probability $\eta_2/(\eta_1+\eta_2)$, and the random walks stops once it reaches the horizontal or vertical axis. For any path from (n,m) to (k,0) , $1 \geq k \geq n$, it must reach (k,1) first before it makes a final move to (k,0). Furthermore, all the paths going from (n,m) to (k,1) must have exactly n-k lefts and m-1 downs, whence the total number of such paths is $\binom{n-k+m-1}{m-1}$. Similarly the total number of paths from (n,m) to (0,l) , $1 \geq l \geq m$, is $\binom{n-l+m-1}{n-1}$. Thus

$$A(n,m) =^d \left\{ \begin{array}{ll} \sum_{i=1}^k \xi_i & \text{with probability } \binom{n-k+m-1}{m-1}(\frac{\eta_1}{\eta_1+\eta_2})^{n-k}(\frac{\eta_2}{\eta_1+\eta_2})^m, k = 1, ..., n \\ -\sum_{i=1}^l \xi_i & \text{with probability } \binom{n-l+m-1}{n-1}(\frac{\eta_1}{\eta_1+\eta_2})^{n}(\frac{\eta_2}{\eta_1+\eta_2})^{m-l}, l = 1, ..., m \end{array} \right\}.$$

and the lemma is proven.

Now, let's prove the proposition B.1. By the same analogy used in Lemma B.1 to compute probability $P_{n,m}, 1 \geq k \geq n$, the probability weight assigned to $\sum_{i=1}^k \xi_i^+$ when we decompose $\sum_{i=1}^k Y_i$, it is equivalent to consider the probability of the random walk ever reach (k,0) starting from the point (i,n-i) being $\binom{n}{i} p^i q^{n-i}$. Note that the point (k,0) can only be reached from point (i,n-i) such that $k \geq i \geq n-1$, because the random walk can only go left or down, and stops once it reaches the horizontal axis. Therefore, for $1 \geq k \geq n-1$, (B3) leads to

$$P_{n,k} = \sum_{i=k} n - 1 P(goingfrom(i, n-i)to(k,0)).P(startingfrom(i, n-i))$$

$$= \sum_{i=k}^{n-1} \binom{i + (n-i) - k - 1}{(n-i) - 1} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{i-k} (\frac{\eta_2}{\eta_1+\eta_2})^{n-i} p^i q^{n-i}$$

$$= \sum_{i=k}^{n-1} \binom{n-k-1}{n-i-1} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{i-k} (\frac{\eta_2}{\eta_1+\eta_2})^{n-i} p^i q^{n-i}$$

$$= \sum_{i=k}^{n-1} \binom{n-k-1}{i-k} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{i-k} (\frac{\eta_2}{\eta_1+\eta_2})^{n-i} p^i q^{n-i}$$

Of course $P_{n,n} = p^n$. Similarly, we can compute $Q_{n,k}$:

$$Q_{n,k} = \sum_{i=k} n - 1 P(goingfrom(n-i, i)to(0,k)).P(startingfrom(n-i, i))$$

$$= \sum_{i=k}^{n-1} \binom{i + (n-i) - k - 1}{(n-i) - 1} \binom{n}{n-i} (\frac{\eta_1}{\eta_1+\eta_2})^{n-i} (\frac{\eta_2}{\eta_1+\eta_2})^{i-k} p^{n-i} q^{i}$$

$$= \sum_{i=k}^{n-1} \binom{n-k-1}{i-k} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{n-i} (\frac{\eta_2}{\eta_1+\eta_2})^{i-k} p^{n-i} q^i$$

with $Q_{n,n} = q^n$. Incidentally, we have also got $\sum k = 1n(P_{n,k} + Q_{n,k}) = 1$

B.2. Let's develop now the results on Hh functions. First of all, note that $Hh_n(x) \to 0$, as $x \to \infty$, for $n \geq -1$; and $Hh_n(x) \to \infty$, as $x \to -\infty$, for $n \geq -1$; and $Hh_0(x) = \sqrt{2\pi}\phi(-x) \to \sqrt{2\pi}$, as $x \to -\infty$. Also, for every $n \geq -1$, as $x \to \infty$,

$$lim Hh_n(x)/\{\frac{1}{x^{n+1}} e^{-\frac{x^2}{2}}\} = 1$$

and as $x \to \infty$

$$Hh_n(x) = O(|x|^n)$$

Here (B4) is clearly true for $n = -1$, while for $n \geq 0$ note that as $x \to_\infty$,

$$Hh_n(x) = \frac{1}{n!} \int_x \infty (t-x)^n e^{-\frac{t^2}{2}} dt$$

$$\leq \frac{2^n}{n!} \int_{-\infty}^{\infty} |t|^n e^{-t^2} 2dt + \frac{2^n}{n!} \int -\infty\infty |x|^n e^{-t^2} 2dt = O(|x|^n)$$

For option pricing it is important to evaluate the integral $I_n(c; \alpha; \beta; \delta)$,

$$I_n(c; \alpha; \beta; \delta) = \int_c \infty e^{\alpha x} Hh_n(\beta x - \delta) dx, n \geq 0$$

for arbitrary constants α, c and β.

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BIOGRAPHICAL SKETCH

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