Time-dependent Perturbation Theory [1]

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[1] extended notes from the class of Dr. Bernido

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an extended lecture notes from my graduate class on Quantum Mechanics, added some topics not covered during the class. Detailed calculations are added for future reference and to make the life of the reader easier. Life is too short.

In quantum mechanics, **perturbation theory** is a set of approximation schemes directly related to mathematical perturbation for describing a complicated quantum system in terms of a simpler one. The idea is to start with a simple system for which a mathematical solution is known, and add an additional "perturbing" Hamiltonian representing a weak disturbance to the system. If the disturbance is not too large, the various physical quantities associated with the perturbed system (e.g. its energy levels and eigenstates) can be expressed as "corrections" to those of the simple system. [3]

[3] copied from wiki, I like this definition of perturbation theory, it emphasizes the idea that complicated systems can be studied by examining the simpler ones

Hamiltonian Approximations

Perturbation theory is an important tool for describing real quantum systems, as it turns out to be very difficult to find exact solutions to the Schrodinger equation for Hamiltonians of even moderate complexity. The Hamiltonians to which we know exact solutions, such as the hydrogen atom, the quantum harmonic oscillator and the particle in a box, are too idealized to adequately describe most systems. Using perturbation theory, we can use the known solutions of these simple Hamiltonians to generate solutions for a range of more complicated systems.[4]

[4] copied from wiki again!

Time-independent Perturbation Theory

Consider the Hamiltonian,

$$H = H_0 + H_1 \tag{1}$$

where the perturbing Hamiltonian is explicitly time-dependent,

$$H_1 = H_1(t)$$

e.g. $H_1 = cos(\omega t), H_1 = \exp(-i\omega t)$

From the Schrodinger equation, [5]

$$H\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} \tag{2}$$

[5] $\Psi(\mathbf{r},t)$ is the wavefunction of the unperturbed Hamiltion H_0

$$\underbrace{(H_0 + H_1)}_{H} \Psi(\mathbf{r}, t) = i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} \tag{3}$$

We worked with the unperturbed solutions of the time-independent eigenvalue equation.

$$H_0 \Psi_n^0 = E_n \Psi_n^0 \tag{4}$$

where ψ_n^0 form a complete orthonormal sets!

We let $\Psi(t)$ be the state of the perturbed system at time t. We can make the expansion: [6]

[6] $\Psi(t)$ is wavefunction of the perturbed Hamiltion $H = H_0 + H_1$

$$\Psi(t) = \sum_n c_n(t) \exp(-i\omega_n t) \Psi_n^0 \tag{5}$$

where $\omega_n = E_n/\hbar$ (an energy eigenvalue of the unperturbed Hamiltonian H_0), and $|c_n(t)|^2$ is the probability of finding the system in the state $|n\rangle$ at time t.

The time-dependent wavefunction obeys the Schrodinger equation,

$$\underbrace{(H_0 + H_1)}_{H} \Psi(t) = i\hbar \frac{\partial \Psi(t)}{\partial t} \tag{6}$$

We then substitute equation (5) to equation (6),

$$\begin{aligned}
&(H_0 + H_1) \sum c_n(t) \exp(-i\omega_n t) \left|\Psi_n^0\right\rangle \\
&\qquad = i\hbar \frac{\partial}{\partial t} \left(\sum c_n(t) \exp(-i\omega_n t) \left|\Psi_n^0\right\rangle\right) \\
&H_0 \sum c_n(t) \exp(-i\omega_n t) \left|\Psi_n^0\right\rangle + H_1 \sum c_n(t) \exp(-i\omega_n t) \left|\Psi_n^0\right\rangle \\
&\qquad = i\hbar \sum_n \left((-i\omega_n t) \exp(-i\omega_n t) \left|\Psi_n^0\right\rangle + \frac{dc_n}{dt} \exp(-i\omega_n t) \left|\Psi_n^0\right\rangle \right)
\end{aligned}$$

We then multiply the results with $\langle \Psi_m^0 |$ (on the left side), [7]

[7] please note we've shifted to Dirac notation

$$\begin{aligned}
&\left\langle \Psi_m^0 \right| H_0 \sum c_n(t) \exp(-i\omega_n t) \left|\Psi_n^0\right\rangle + \left\langle \Psi_m^0 \right| H_1 \sum c_n(t) \exp(-i\omega_n t) \left|\Psi_n^0\right\rangle \\
&= i\hbar \sum_n \left((-i\omega_n t) \exp(-i\omega_n t) \left\langle \Psi_m^0 | \Psi_n^0 \right\rangle + \frac{dc_n}{dt} \exp(-i\omega_n t) \left\langle \Psi_m^0 | \Psi_n^0 \right\rangle \right) \\
&\sum c_n(t) \exp(-i\omega_n t) \left\langle \Psi_m^0 \right| H_0 \left|\Psi_n^0\right\rangle + \sum c_n(t) \exp(-i\omega_n t) \left\langle \Psi_m^0 \right| H_1 \left|\Psi_n^0\right\rangle \\
&= i\hbar \sum_n \left((-i\omega_n t) \exp(-i\omega_n t) \left\langle \Psi_m^0 | \Psi_n^0 \right\rangle + \frac{dc_n}{dt} \exp(-i\omega_n t) \left\langle \Psi_m^0 | \Psi_n^0 \right\rangle \right)
\end{aligned}$$

To simplify the equation, we use equation (4), the definition of ω_n and the orthonormality of the wavefunctions, [8]

[8] use orthonormality equation: $\langle \Psi_m^0 | \Psi_n^0 \rangle = \delta_{mn}$

$$\cancel{\sum E_n c_n(t) \exp(-i\omega_n t)\delta_{mn}} + \sum c_n(t) \exp(-i\omega_n t) \langle \Psi_m^0 | H_1 | \Psi_n^0 \rangle = \cancel{\sum E_n c_n(t) \exp(-i\omega_n t)\delta_{mn}} + i\hbar \sum \frac{dc_n}{dt} \exp(-i\omega_n t)\delta_{mn}$$

$$\sum c_n(t) \exp(-i\omega_n t) \langle \Psi_m^0 | H_1 | \Psi_n^0 \rangle = i\hbar \sum \frac{dc_n}{dt} \exp(-i\omega_n t)\delta_{mn}$$

Manipulating the equation above, we have:

$$\frac{dc_m}{dt} = -\frac{i}{\hbar} \sum_n c_n(t) \langle m | H_1 | n \rangle \exp(-i(\omega_m - \omega_n)t) \tag{7}$$

This exact results enables us to determine the time dependence of the coefficients $c_n(t)$ and the wavefunctions.

$$c_m(t) = -\frac{i}{\hbar} \sum_n \int_0^t c_n(t) \langle m | H_1 | n \rangle e^{(-i(\omega_m - \omega_n)t)} dt \tag{8}$$

Several important results follows from this, such as **Fermi's Golden Rule** which relates the rate of transitions between quantum states to the density of states at particular energies.

If H_1 is small,

$$\frac{dc_n}{dt} << 1$$

at $t = 0$, at state $|n\rangle$, we have $c_n(0) = 1$ and for all $c_m = 0; m \neq n$. We can rewrite equation (8) as,

$$c_m(t) \approx -\frac{i}{\hbar} \int_0^t \langle m|H_1|n\rangle \, e^{-i(\omega_m - \omega_n)t} \underbrace{c_n(0)}_{1} dt \tag{9}$$

Special Cases

CASE 1:

Suppose the perturbation has acted for finite duration, $t = 0$ to $t = \tau$. This means,

Page Layout

Headings

This style provides A- and B-heads (that is, `\section` and `\subsection`), demonstrated above.

The Tufte-LaTeX classes will emit an error if you try to use `\subsubsection` and smaller headings.

In his later books,[9] Tufte starts each section with a bit of vertical space, a non-indented paragraph, and sets the first few words of the sentence in small caps. To accomplish this using this style, use the `\newthought` command:

[9] Edward R. Tufte. *Beautiful Evidence.* Graphics Press, LLC, first edition, May 2006. ISBN 0-9613921-7-7

```
\newthought{In his later books}, Tufte starts...
```

Sidenotes

One of the most prominent and distinctive features of this style is the extensive use of sidenotes. There is a wide margin to provide ample room for sidenotes and small figures. Any `\footnotes` will automatically be converted to sidenotes.[10] If you'd like to place ancillary information in the margin without the sidenote mark (the superscript number), you can use the `\marginnote` command.

[10] This is a sidenote that was entered using the `\footnote` command.

This is a margin note. Notice that there isn't a number preceding the note, and there is no number in the main text where this note was written.

The specification of the `\sidenote` command is:

`\sidenote[`⟨*number*⟩`][`⟨*offset*⟩`]{`*Sidenote text.*`}`

Both the ⟨*number*⟩ and ⟨*offset*⟩ arguments are optional. If you provide a ⟨*number*⟩ argument, then that number will be used as the sidenote number. It will change of the number of the current sidenote only and will not affect the numbering sequence of subsequent sidenotes.

Sometimes a sidenote may run over the top of other text or graphics in the margin space. If this happens, you can adjust the vertical position of the sidenote by providing a dimension in the ⟨*offset*⟩ argument. Some examples of valid dimensions are:

```
1.0in    2.54cm    254mm    6\baselineskip
```

If the dimension is positive it will push the sidenote down the page; if the dimension is negative, it will move the sidenote up the page.

While both the ⟨*number*⟩ and ⟨*offset*⟩ arguments are optional, they must be provided in order. To adjust the vertical position of the sidenote while leaving the sidenote number alone, use the following syntax:

`\sidenote[][`⟨*offset*⟩`]{`*Sidenote text.*`}`

The empty brackets tell the `\sidenote` command to use the default sidenote number.

If you *only* want to change the sidenote number, however, you may completely omit the ⟨*offset*⟩ argument:

`\sidenote[`⟨*number*⟩`]{`*Sidenote text.*`}`

The `\marginnote` command has a similar *offset* argument:

`\marginnote[`⟨*offset*⟩`]{`*Margin note text.*`}`

References

References are placed alongside their citations as sidenotes, as well. This can be accomplished using the normal `\cite` command.[11]

[11] The first paragraph of this document includes a citation.

The complete list of references may also be printed automatically by using the `\bibliography` command. (See the end of this document for an example.) If you do not want to print a bibliography at the end of your document, use the `\nobibliography` command in its place.

To enter multiple citations at one location,[12] you can provide a list of keys separated by commas and the same optional vertical offset argument: `\cite{Tufte2006,Tufte1990}`.

`\cite[`⟨*offset*⟩`]{`*bibkey1*,*bibkey2*,...`}`

[12] Edward R. Tufte. *Beautiful Evidence*. Graphics Press, LLC, first edition, May 2006. ISBN 0-9613921-7-7; and Edward R. Tufte. *Envisioning Information*. Graphics Press, Cheshire, Connecticut, 1990. ISBN 0-9613921-1-8

Figures and Tables

Images and graphics play an integral role in Tufte's work. In addition to the standard figure and tabular environments, this style provides special figure and table environments for full-width floats.

Full page–width figures and tables may be placed in figure* or table* environments. To place figures or tables in the margin, use the marginfigure or margintable environments as follows (see figure 1):

```
\begin{marginfigure}
  \includegraphics{helix}
  \caption{This is a margin figure.}
\end{marginfigure}
```

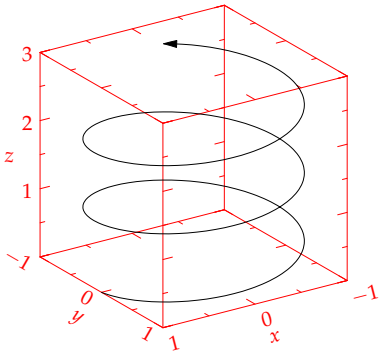

Figure 1: This is a margin figure. The helix is defined by $x = \cos(2\pi z)$, $y = \sin(2\pi z)$, and $z = [0, 2.7]$. The figure was drawn using Asymptote (`http://asymptote.sf.net/`).

The marginfigure and margintable environments accept an optional parameter ⟨*offset*⟩ that adjusts the vertical position of the figure or table. See the "Sidenotes" section above for examples. The specifications are:

```
\begin{marginfigure}[⟨offset⟩]
   ...
\end{marginfigure}

\begin{margintable}[⟨offset⟩]
   ...
\end{margintable}
```

Figure 2 is an example of the `figure*` environment and figure 3 is an example of the normal `figure` environment.

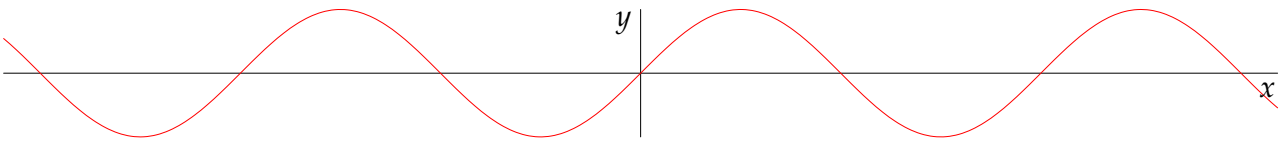

Figure 2: This graph shows $y = \sin x$ from about $x = [-10, 10]$. *Notice that this figure takes up the full page width.*

Table 1 shows table created with the `booktabs` package. Notice the lack of vertical rules—they serve only to clutter the table's data.

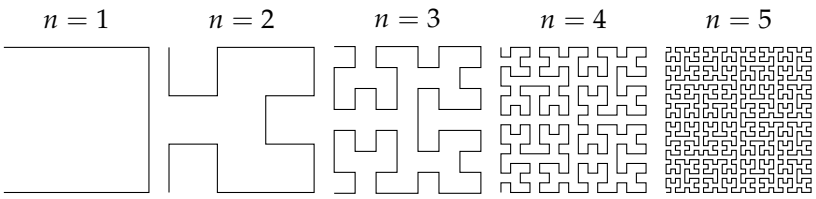

Figure 3: Hilbert curves of various degrees n. *Notice that this figure only takes up the main textblock width.*

Margin	Length
Paper width	8 1/2 inches
Paper height	11 inches
Textblock width	6 1/2 inches
Textblock/sidenote gutter	3/8 inches
Sidenote width	2 inches

Table 1: Here are the dimensions of the various margins used in the Tufte-handout class.

Full-width text blocks

In addition to the new float types, there is a fullwidth environment that stretches across the main text block and the sidenotes area.

```
\begin{fullwidth}
Lorem ipsum dolor sit amet...
\end{fullwidth}
```

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

Typography

Typefaces

If the Palatino, Helvetica, and `Bera Mono` typefaces are installed, this style will use them automatically. Otherwise, we'll fall back on the Computer Modern typefaces.

Letterspacing

This document class includes two new commands and some improvements on existing commands for letterspacing.

When setting strings of ALL CAPS or SMALL CAPS, the letterspacing—that is, the spacing between the letters—should be increased slightly.[13] The `\allcaps` command has proper letterspacing

[13] Robert Bringhurst. *The Elements of Typography*. Hartley & Marks, 3.1 edition, 2005. ISBN 0-88179-205-5

for strings of FULL CAPITAL LETTERS, and the `\smallcaps` command has letterspacing for SMALL CAPITAL LETTERS. These commands will also automatically convert the case of the text to upper- or lowercase, respectively.

The `\textsc` command has also been redefined to include letterspacing. The case of the `\textsc` argument is left as is, however. This allows one to use both uppercase and lowercase letters: THE INITIAL LETTERS OF THE WORDS IN THIS SENTENCE ARE CAPITALIZED.

Installation

To install the Tufte-LaTeX classes, simply drop the following files into the same directory as your `.tex` file:

```
tufte-common.def
tufte-handout.cls
tufte-book.cls
```

More Documentation

For more documentation on the Tufte-LaTeX document classes (including commands not mentioned in this handout), please see the sample book.

Support

The website for the Tufte-LaTeX packages is located at `http://code.google.com/p/tufte-latex/`. On our website, you'll find links to our SVN repository, mailing lists, bug tracker, and documentation.

References

Robert Bringhurst. *The Elements of Typography*. Hartley & Marks, 3.1 edition, 2005. ISBN 0-88179-205-5.

Edward R. Tufte. *Envisioning Information*. Graphics Press, Cheshire, Connecticut, 1990. ISBN 0-9613921-1-8.

Edward R. Tufte. *Beautiful Evidence*. Graphics Press, LLC, first edition, May 2006. ISBN 0-9613921-7-7.