High Quality Typesetting *MATHEMATICA*® Sessions with LaTeX

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1. *MATHEMATICA*® and LaTeX

- the FrontEnd is already a typesetting engine for screen oriented documents with out pages, foot-notes, multi column typesetting
- `TeXSave[]` force the usage of two macro package wrisym.sty for the *MATHEMATICA*® fonts and notebook2e.sty for the page layout. The notebook2e.sty is too restrictive.
  - no export of the style sheet used
  - "macros" will be not preserved – instead the boxes used by the FrontEnd are expanded. The markup structure of the document is destroyed
- `TeXSave[]` can't export tables.
- hyperlinks are not exported
- almost no support for table of contents, and index generation
- almost not support for literature data bases and reference styles
- automatic translation *MATHEMATICA*® $\longrightarrow$ LaTeXis almost impossible

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2. Why Should a Computer Algebra Care for the Document Layout ?

For the computer algebra only two document structures are important

- user input
  - visible input
  - hidden input
- output generated by *MATHEMATICA*®
  - mathematical expressions
  - graphics

2.1. Why Hidden Input?

The *MATHEMATICA*® session may include options settings, format definitions and other information that are send to *MATHEMATICA*® but unimportant for the contents of the document. These information should be not visible in the final document.

One may use the output of *MATHEMATICA*® in a document without showing the confusing input.

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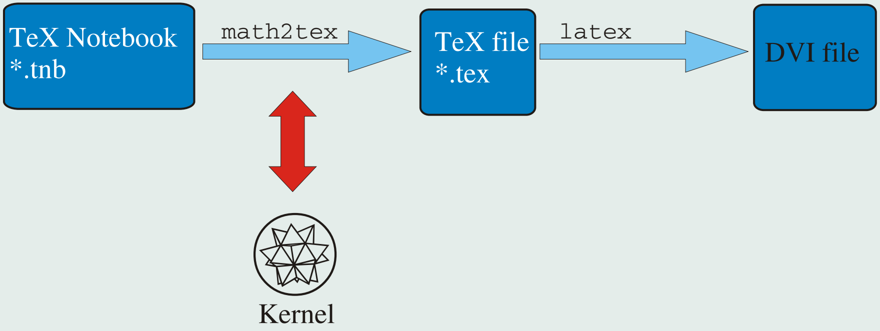
3. math2tex a LaTeX FrontEnd

Since the original *MATHEMATICA*® FrontEnd can't save the full document layout a extra frontend is needed.

- input should send to *MATHEMATICA*®
- output should inserted into the final LaTeXdocument
- the input syntax should be translated into LaTeXto match the original FrontEnd syntax, i. e., `:>` should be translated to $:\rightarrow$.
- special characters like `\[Alpha]` and `\[DoubleStruckD]` should be usable
- formatting should be automatically translated `D[f[x],x]` to $\partial_x \mathtt{f[x]}$ and `Integrate[f[x],x]` to $\int \mathtt{f[x]}\, \mathbb{d}\mathtt{x}$
- creation of an index for variables used in the input cells
- ignore all other LaTeX commands and environments
- labels to output cells, so that the results of *MATHEMATICA*® computations can be referenced in the text.
- indexed variables like `\Subscript[x,1]` should be formatted as $\mathtt{x}_1$
- extract the input from the LaTeX notebooks to a "true" *MATHEMATICA*® notebook

4. Control Structures



4.1. The `mathinput` environment

The contents is send to *MATHEMATICA®* and shown in the output. The syntax is basically *MATHEMATICA®*'s `InputForm[]`.

```
\begin{mathinput}{A comment.}
Integrate[ psi[x^2] f[x*epsilon] Sqrt[x], x]
\end{mathinput}
```

In[1]:=

$$\int \psi[x^2]\ f[x * \epsilon]\ \sqrt{x}\, dx$$

A comment.

Out[1]=

$$\int \sqrt{x} f(x\epsilon)\psi\left(x^2\right)\, dx$$

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4.2. The `mathhidden` environment

The contents of the `mathhidden` environment is not shown but if the result is *not* `Null` the output is inserted into the LaTeXfile. In this way we can talk about the Schrödinger equation

$$i\hbar\psi^{(0,1)}(x,t) = \mathcal{H}(\psi)(x,t) \tag{1}$$

without typing the TeX code of the formula. The document contain only the code:

```
\begin{mathhidden}[Eqn::sg1]
I hbar D[psi[x,t],t]==scH[psi][x,t]
\end{mathhidden}
```

In[2]:=

$$\partial_{x,x}\,f[x,y]$$

Out[2]=

$$f^{(2,0)}(x,y)$$

Both environments can have an optional argument with a label for the *MATHEMATICA*® output.

5. Graphics

Graphics is saved as PostScript but *not* automatically inserted into the LaTeX output, because one may have a caption for the graphics and LaTeX should have the freedom to place the float.

Labels in graphics objects need the psfrag LaTeXstyle to typeset axes labels. The kernel alone knows nothing about the metrics of the fonts and can not place the characters in a PostScript graphics. Only the true FrontEnd read the font information and the metrics and the kernel calls back to the FrontEnd when a graphics include `Text[]` objects.

6. Symbols

Since the TEX file is 7-bit ASCII the characters like `\[Alpha]` or `\[DoubleStruckCapitalD]` entered by the alias of the FrontEnd. A names like `\[ExponentialE]` is to long to type it directly. The real FrontEnd use ESC ee ESC to produce e. The TEX frontend uses a symbol table that lists the name used in the TEX notebook, the name for TEX, the name used in *MATHEMATICA*® expressions for that symbol and a sorting key for the index. Private symbol translations can be given in a second symbol table.

```
E       \ee      E        e
I       \ii      I        i
Pi      \pi      Pi       p
hbar    \hbar    \[HBar]  h
```

7. Command Line Options for `math2tex`

`math2tex` *<texnotebook> options*

Table 1: Command line switches

`-o` *output file*	`texnb.tex`	LaTeX output
`-plevel` *integer*	0	parse level for input transformation
`-nb` *notbebook*		FrontEnd notebook
`±` `cm`	`+cm`	call *MATHEMATICA®* to evaluate the input
`-sym` *symbol table*	`.symtab`	general symbol table
`-psym` *symbol table*		private symbol table

Table 2: Parsing levels

parse level	input	LaTeX translation
1	`x^2`	x^2
2	`Sqrt[a+b]`	$\sqrt{a+b}$
4	`D[f[x],x]`	$\partial_x f[x]$
8	`Sum[a[i],{i,0,Infinity}]`	$\sum_{i=0}^{\infty} a[i]$
16	`Integrate[f[x],x]`	$\int f[x] \, dx$
32	`Element[x,Reals]`	$x \in \mathbb{R}$

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8. An Example: Quantum Mechanic Oscillator

No additional correction in the LaTeX output where made.

```
math2tex MathType.tnb -plevel 63 -o MathType.tex
```

The figure was created with the *MATHEMATICA*® FrontEnd because psfrag work only with dvipsdvipdfm and not with pdftex, that is used for the slides.

In[1]:=

```
Hamiltonian[ψ_, x_] :=
  -ℏ^2 ∂_{x,2}ψ/(2μ) +
    k * x^2 * ψ/2
```

Define the Hamiltonian

In[2]:=

```
deqn =
  Hamiltonian[ψ[x], x] ==
     ℰψ[x]
```

Define the stationary Schrödinger equation

Out[2]=

$$\frac{1}{2}kx^2\psi(x) - \frac{\hbar^2\psi''(x)}{2\mu} = \mathcal{E}\psi(x)$$

Now we need dimension less variables.

In[3]:=

```
deqn = Map[
      Simplify[2 * μ * #/ℏ^2] &,
       deqn] /. k → ω^2 * μ
```

The equation must be multiplied by $2\mu/(\hbar^2)$

Out[3]=

$$\frac{x^2\mu^2\omega^2\psi(x)}{\hbar^2} - \psi''(x) = \frac{2\mathcal{E}\mu\psi(x)}{\hbar^2}$$

In[4]:=

```
deqn =
   deqn /. x →
                    ξ * √(ℏ/(μ * ω)) //.
     {ψ[a_ * ξ] :→ ψ[ξ],
      Derivative[n_][f_][a_ * ξ] :→
        a^(-n) * Derivative[n][f][ξ]
      } // Simplify
```

The last rule transform the derivatives of a scaled argument.

Out[4]=

$$\mu\left(\left(\frac{2\mathcal{E}}{\hbar}-\xi^2\omega\right)\psi(\xi)+\omega\psi''(\xi)\right)=0$$

In[5]:=

```
deqn = (ℏ * #/(μ * ω) & /@ deqn) /.
     ℰ →
       ℏ * ω * ϵ/2 //
         Simplify
```

The factor $\hbar/\omega\mu$ cancels and the dimensionless eigenvalue ϵ is inserted.

Out[5]=

$$\hbar\left(\left(\epsilon-\xi^2\right)\psi(\xi)+\psi''(\xi)\right)=0$$

The eigenfunctions must be square integrable

$$\int_{-\infty}^{\infty}\psi^*(\xi)\psi(\xi)\,d\xi<\infty \tag{2}$$

The asymtotic dependence on x should be $|x|- > \infty$ and $\psi(\xi)$ should $\psi(\xi)\propto v(\xi)\exp(-a\xi^2)$. This guarantees that the normalization can be done until $v(\xi)$ grow exponential.

In[6]:=

```
subst = ψ[ξ] → v[ξ] * Exp[-ξ^2/2]
```

The replacement rule for the asymptotic behaviour.

Out[6]=

$$\psi(\xi) \to e^{-\frac{\xi^2}{2}} v(\xi)$$

In[7]:=

```
rules =
  Map[
    {#, ∂_ξ #, ∂_{ξ,2} # } &,
    subst
   ] // Thread;
```

Insert the new function into the differential equation.

In[8]:=

```
deqn1 =
  Cancel[Exp[ξ^2/2] * #] & /@
     (deqn //. rules)
```

Make the replacement for the asymptotic behaviour and cancel $\exp(\xi^2/2)$.

Out[8]=

$$-\hbar\left(-\epsilon v(\xi) + v(\xi) + 2\xi v'(\xi) - v''(\xi)\right) = 0$$

In[9]:=

```
deqn2 = deqn1 /.
    a_ == (b_ /; b ≠ 0) :>
       b - a == 0 //.
    a_. * v[ξ] + b_. * v[ξ] :>
      (a + b) * v[ξ]
```

Collect the factors of $v(\xi)$ and make a homogene equation.

Out[9]=

$$-\hbar\left((1-\epsilon)v(\xi) + 2\xi v'(\xi) - v''(\xi)\right) = 0$$

In[10]:=

```
sol = DSolve[deqn2, v[ξ], ξ]
```

Now `NDSolve[]` can solve the equation.

Out[10]=

$$\left\{\left\{v(\xi) \to c_1 H_{\frac{\epsilon-1}{2}}(\xi) + c_2\, {}_1F_1\left(\frac{1-\epsilon}{4}; \frac{1}{2}; \xi^2\right)\right\}\right\}$$

For a general ϵ the first solution is an error of *MATHEMATICA®*. Only for the case that ϵ is an odd, positive integer one of the solutions is a Hermite polynom. Otherwise the solution can not normalized and the eigenvalue problem can only be solved for $\epsilon = 2n + 1$. The second solution diverges for $\xi \to 0$

In[11]:=

```
sol = Flatten[sol] /. ϵ → 2 * n + 1 /. C[2] →
0 /. C[1] → 𝒩[n]
```

Insert the eigenvalue and replace the integration constant by the normalzation.

Out[11]=

$$\{v(\xi) \to H_n(\xi)\mathcal{N}(n)\}$$

In[12]:=

```
nrule = 𝒩[n_] :→
        (n! 2^n √π)^(-1/2);
```

Insert the normalization and…

Now all the substitutions must be reversed. From $\epsilon = 2n + 1$ the eigenvalues of the harmonic oscillator are given by $\mathcal{E}_n = \hbar\omega(n + 1/2)$.

In[13]:=

```
efunc = ψ[ξ] /. subst /.
               sol /.
               nrule
```

Compute the normalized eigenfunctions.

Figure 1: The first six eigenfunctions and the corresponding probability density

Out[13]=

$$\frac{e^{-\frac{\xi^2}{2}} H_n(\xi)}{\sqrt[4]{\pi}\sqrt{2^n n!}}$$

9. Conclusions

- The TeX frontend is a perfect replacement for the true FrontEnd
- arbitrary styles an be used
- the translation avoid the most TeX errors

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