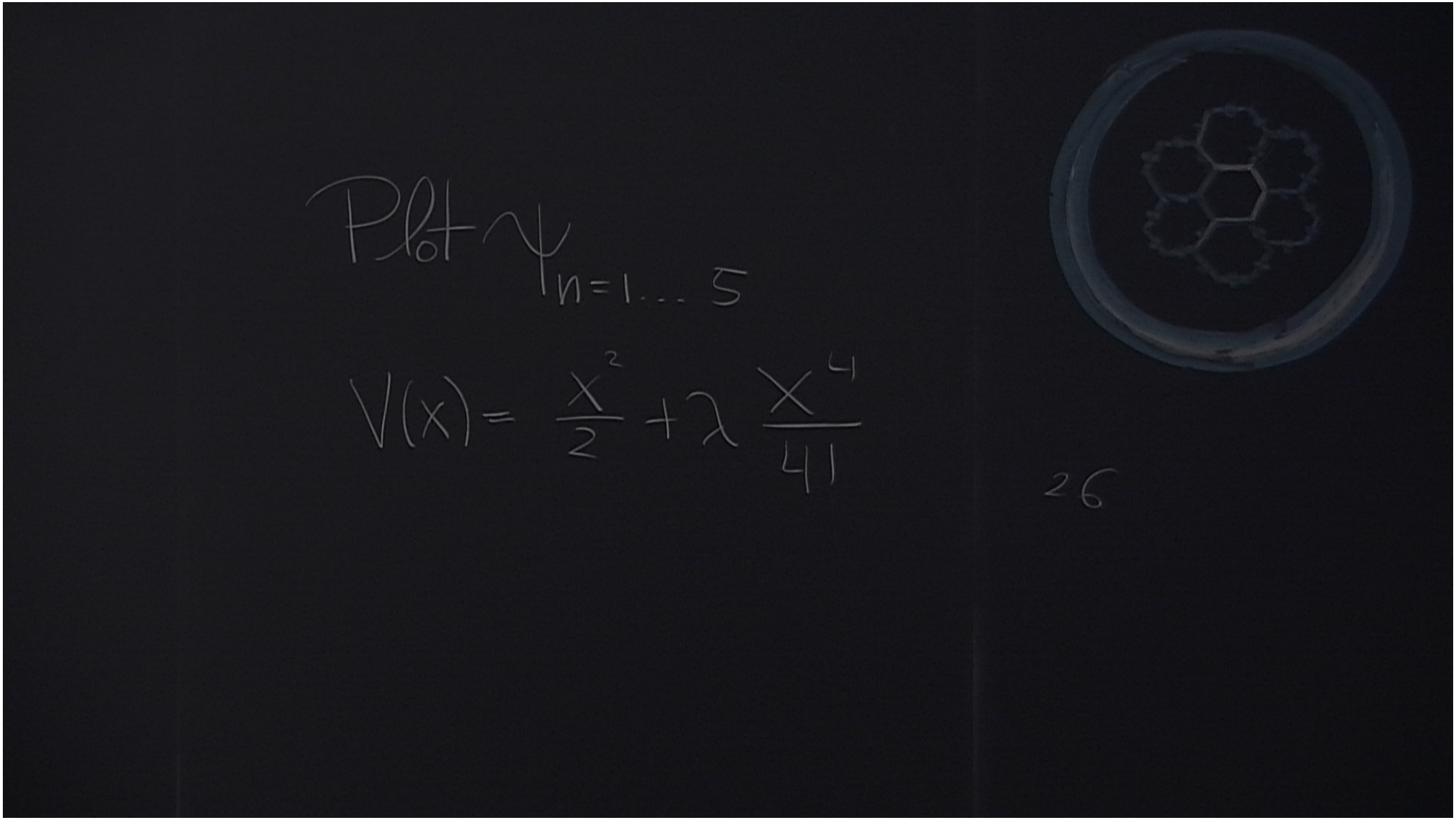
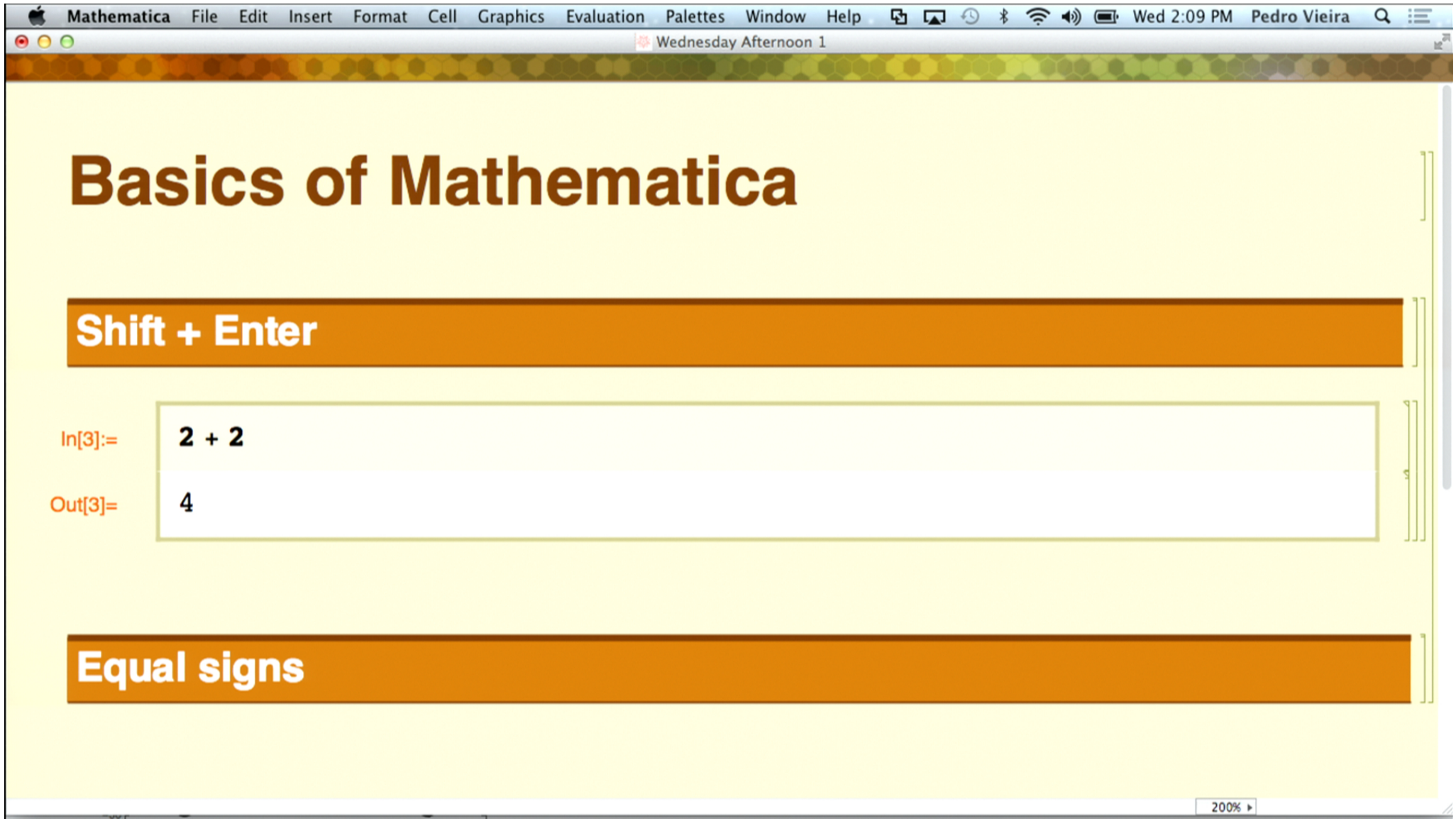
Title: Mathematica Introduction - Pedro Vieira

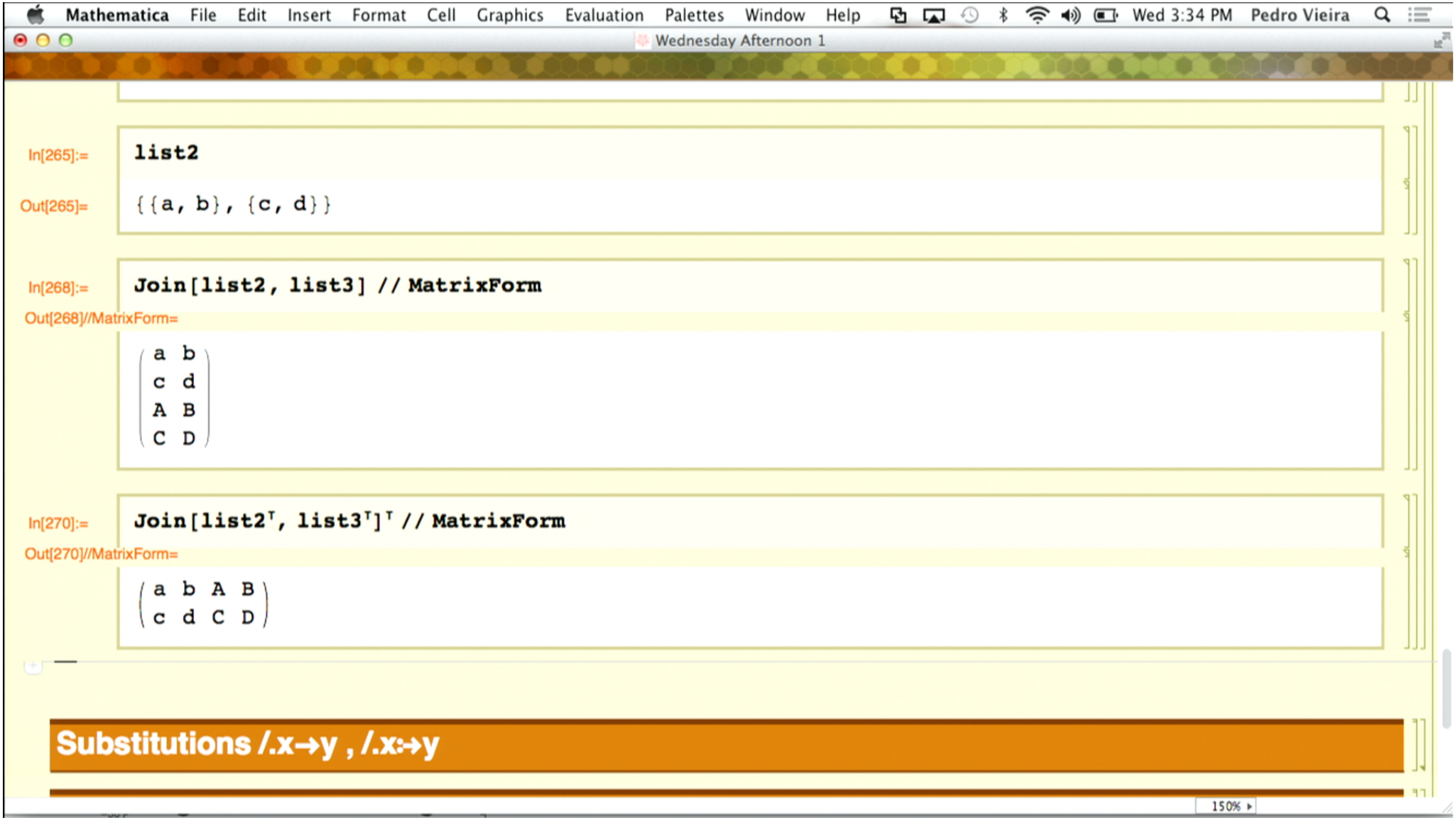
Date: Aug 19, 2015 02:00 PM

URL: http://pirsa.org/15080121

Abstract:


Plot $\psi_{n=1\ldots5}$
$V(x) = \frac{x^2}{2} + \lambda \frac{x^4}{41}$
26


Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 2:09 PM Pedro Vieira
Wednesday Afternoon 1
Basics of Mathematica
Shift + Enter
In[3]:= 2 + 2
Out[3]= 4
Equal signs
200%


Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:34 PM Pedro Vieira
Wednesday Afternoon 1
In[265]:= list2
Out[265]= {{a, b}, {c, d}}
In[268]:= Join[list2, list3] // MatrixForm
Out[268]//MatrixForm=
a b
c d
A B
C D
In[270]:= Join[list2^T, list3^T]^T // MatrixForm
Out[270]//MatrixForm=
a b A B
c d C D
Substitutions /.x→y , /.x:→y
150%

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:36 PM Pedro Vieira

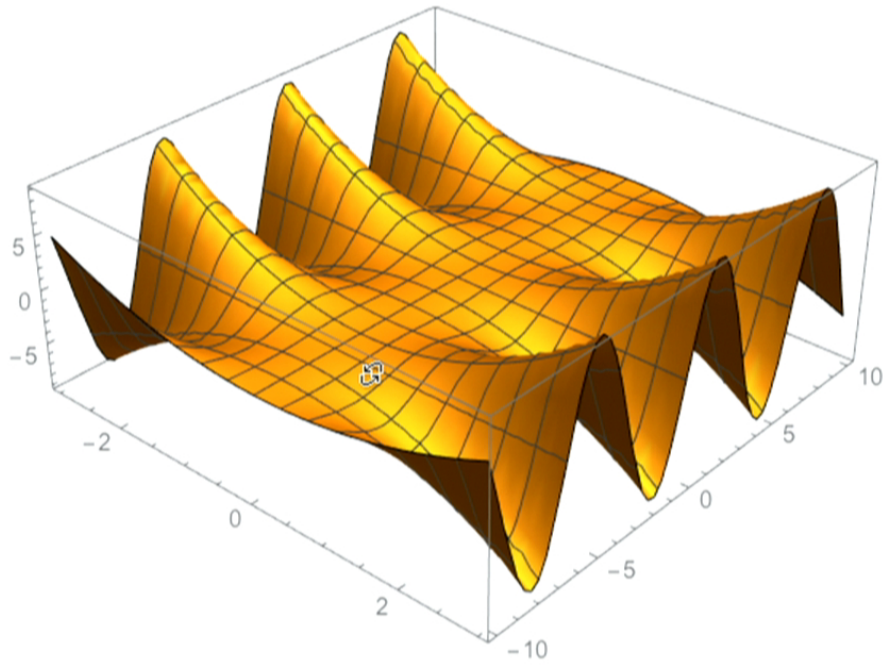
Wednesday Afternoon 1

Simplify[*expr*] performs a sequence of algebraic and other transformations on *expr* and returns the simplest form it finds.
Simplify[*expr*, *assum*] does simplification using assumptions. >>

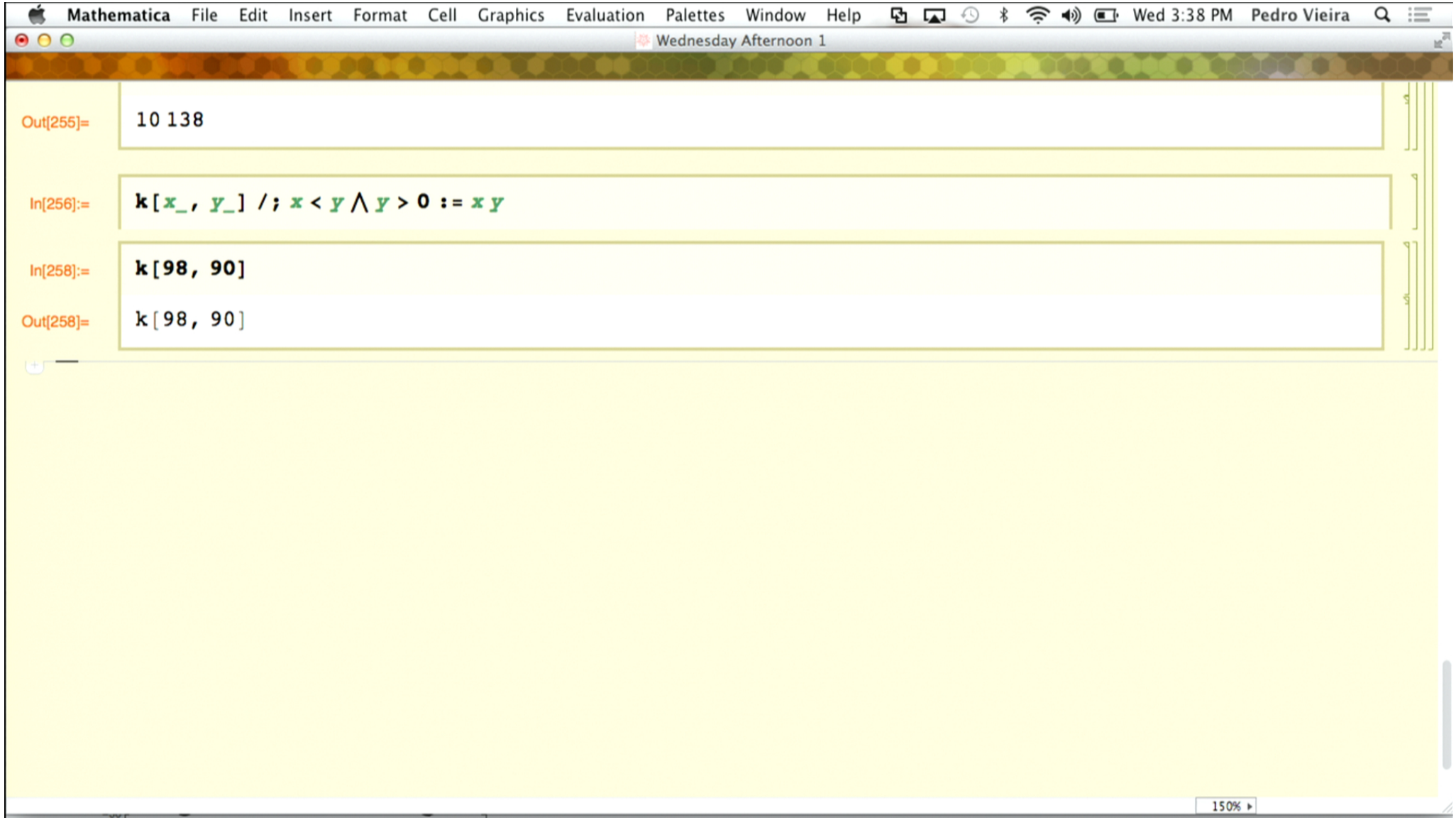
In[271]:=

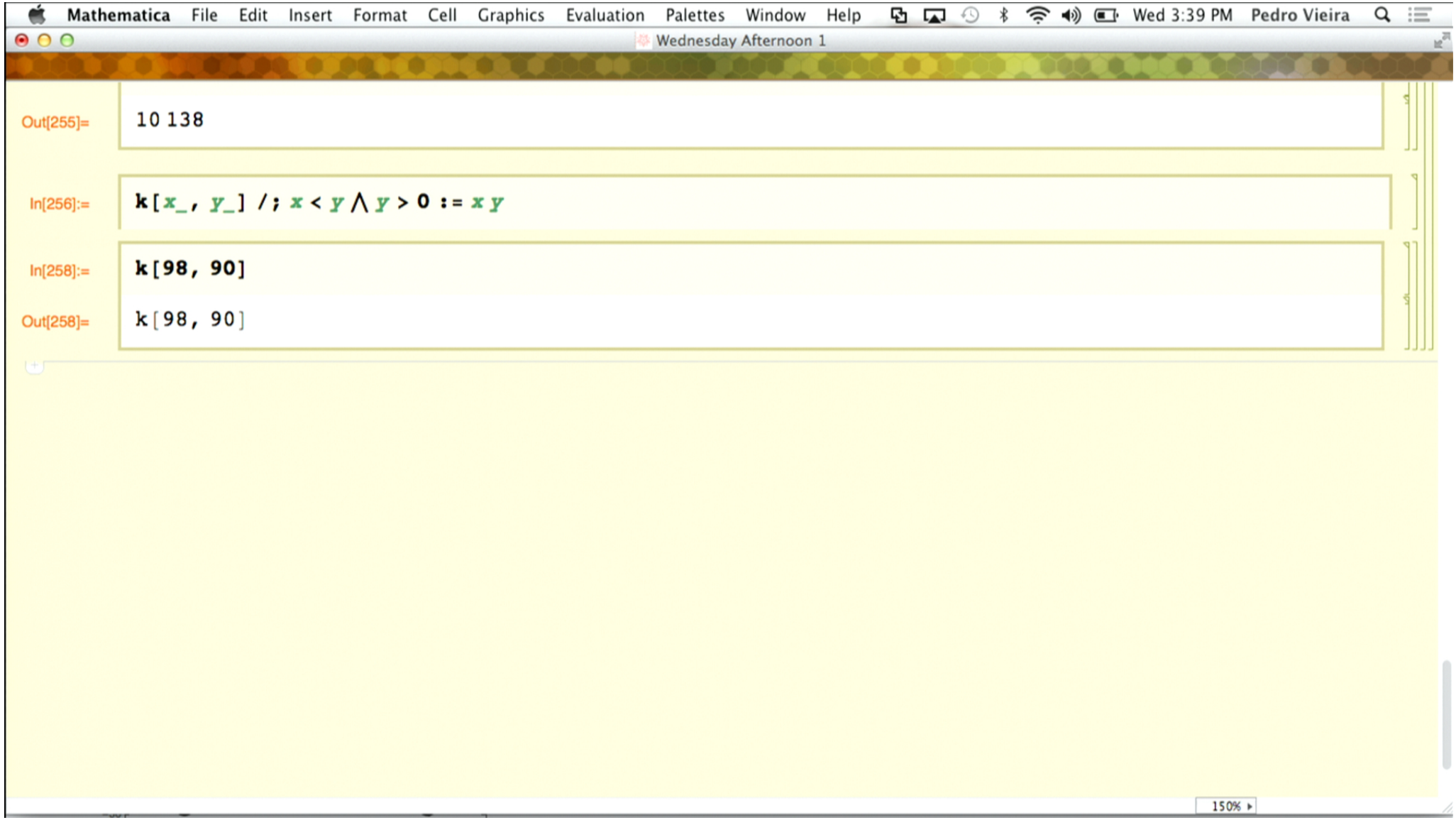
```
Plot3D[x^2 Sin[y], {x, -3, 3}, {y, -10, 10}]
```

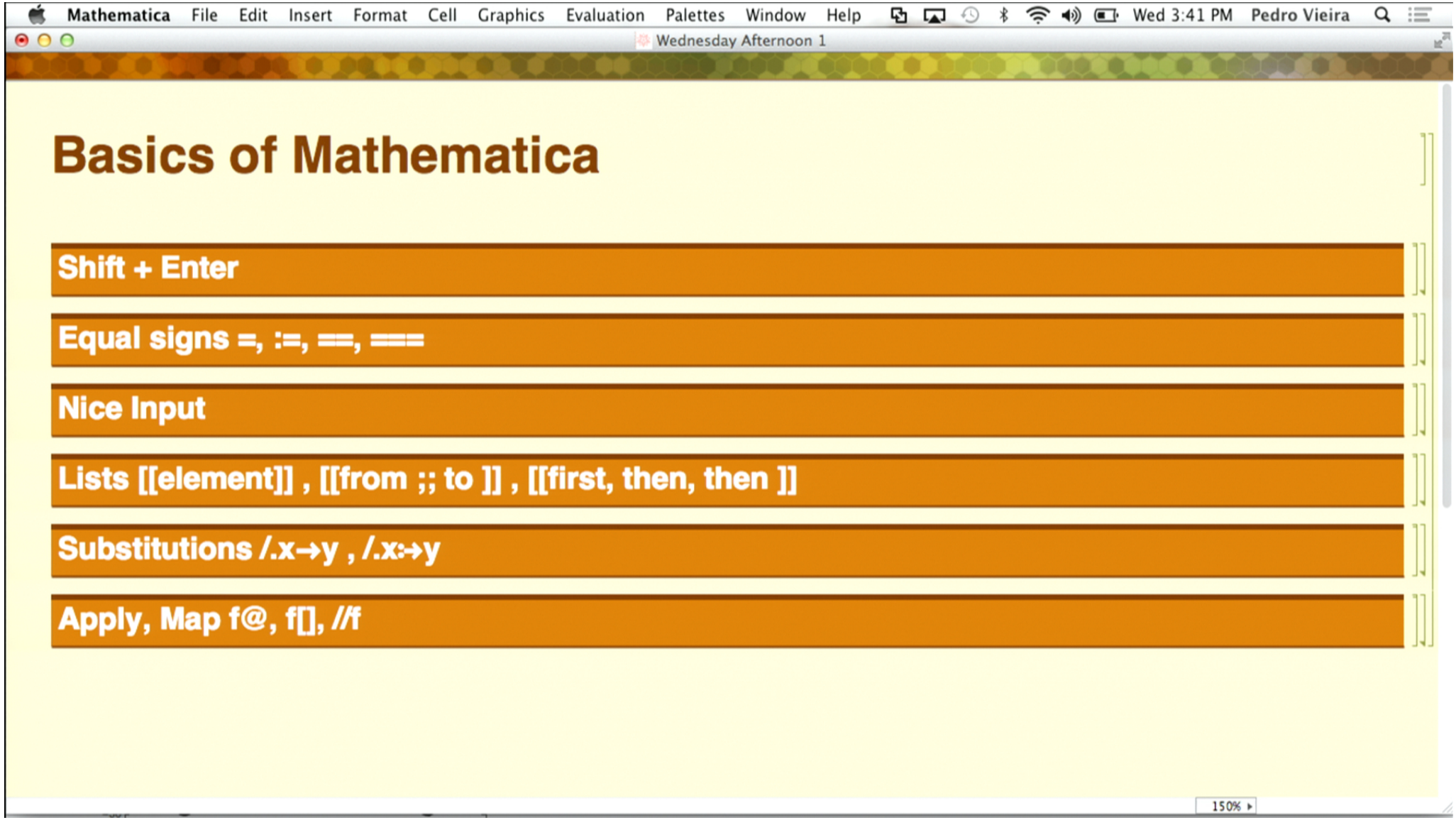
Out[271]=

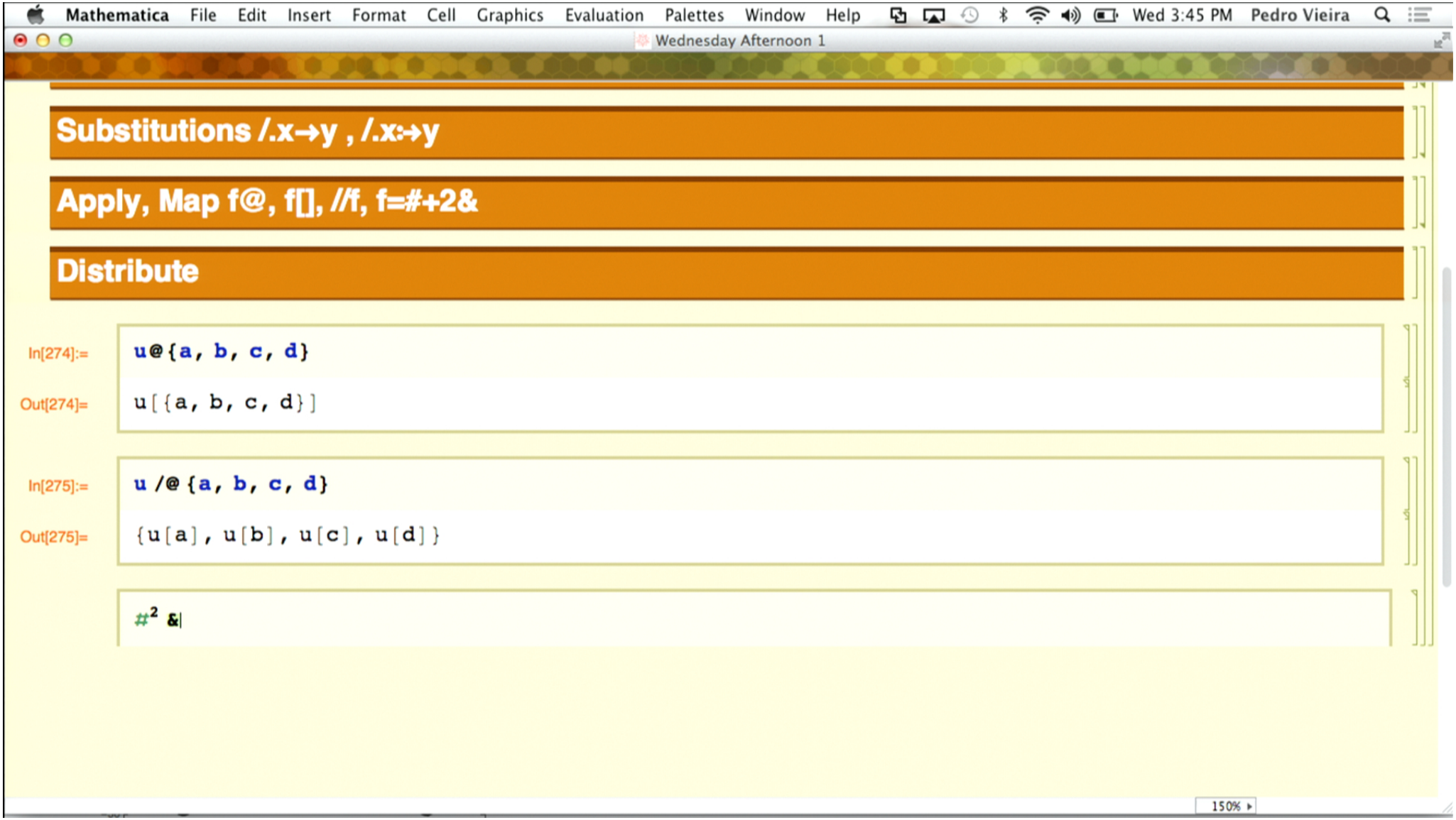


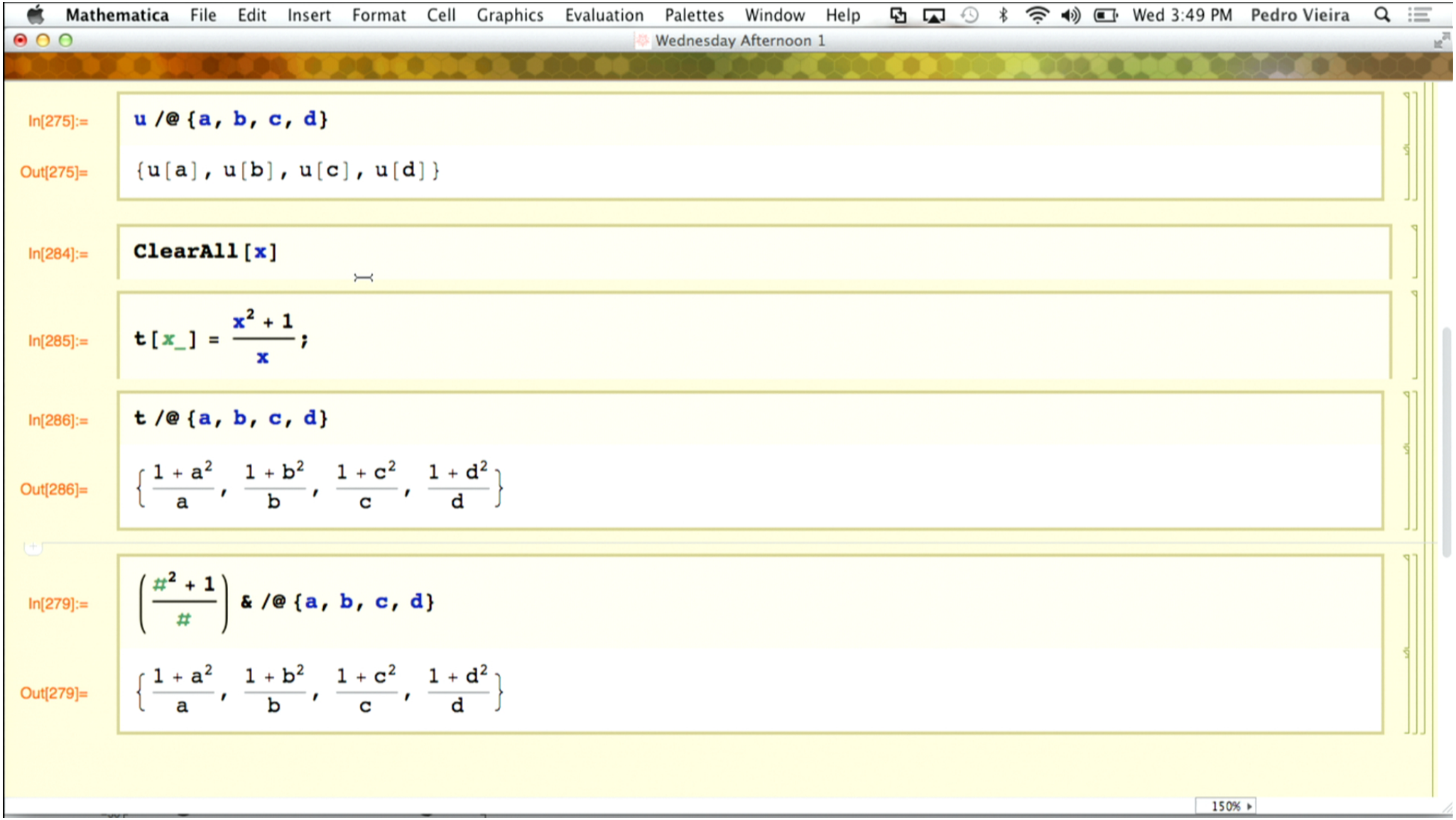
150%

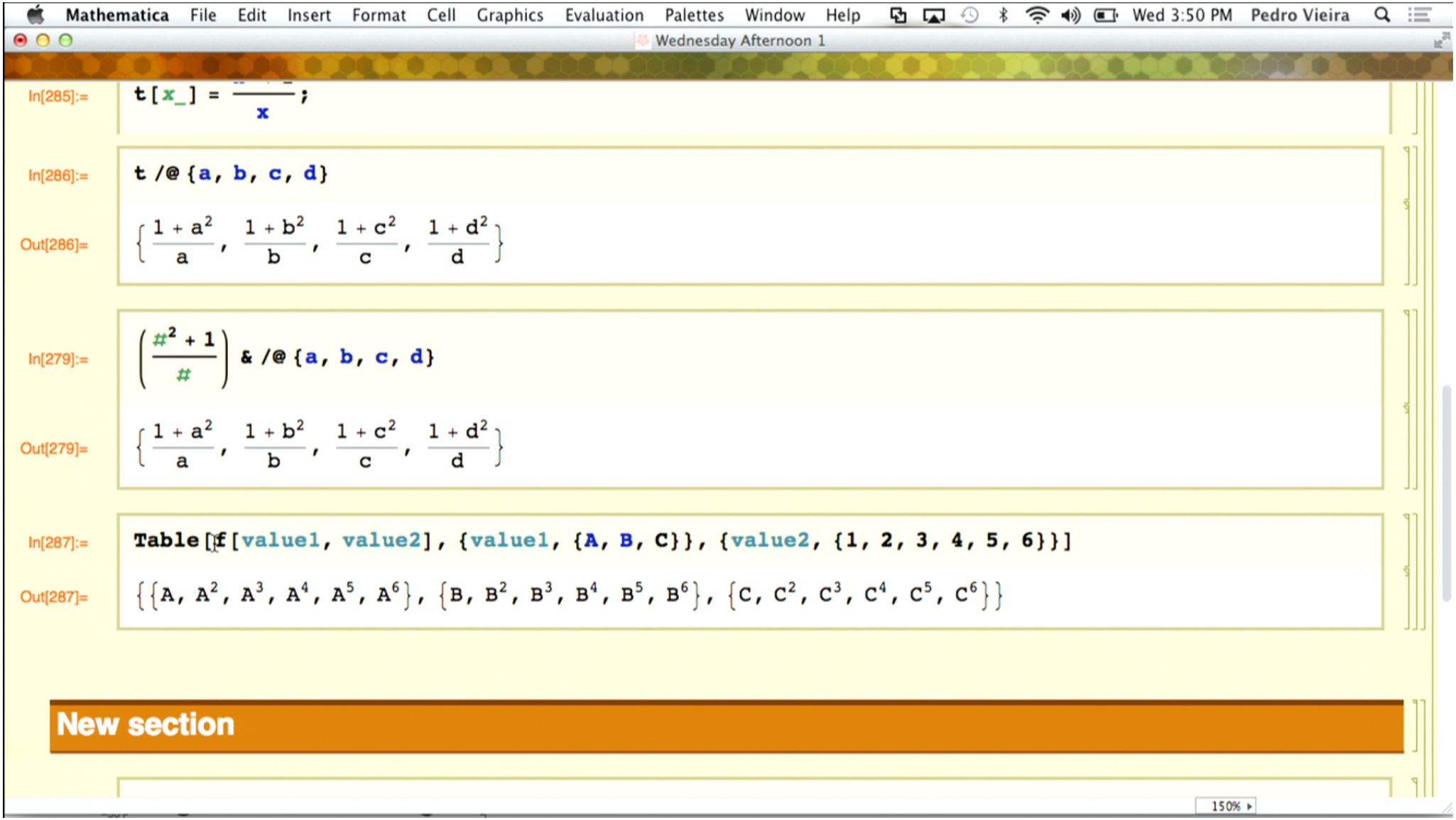

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:38 PM Pedro Vieira
Wednesday Afternoon 1
Out[255]= 10 138
In[256]:= k[x_, y_] /; x < y ∧ y > 0 := x y
In[258]:= k[98, 90]
Out[258]= k[98, 90]
150%

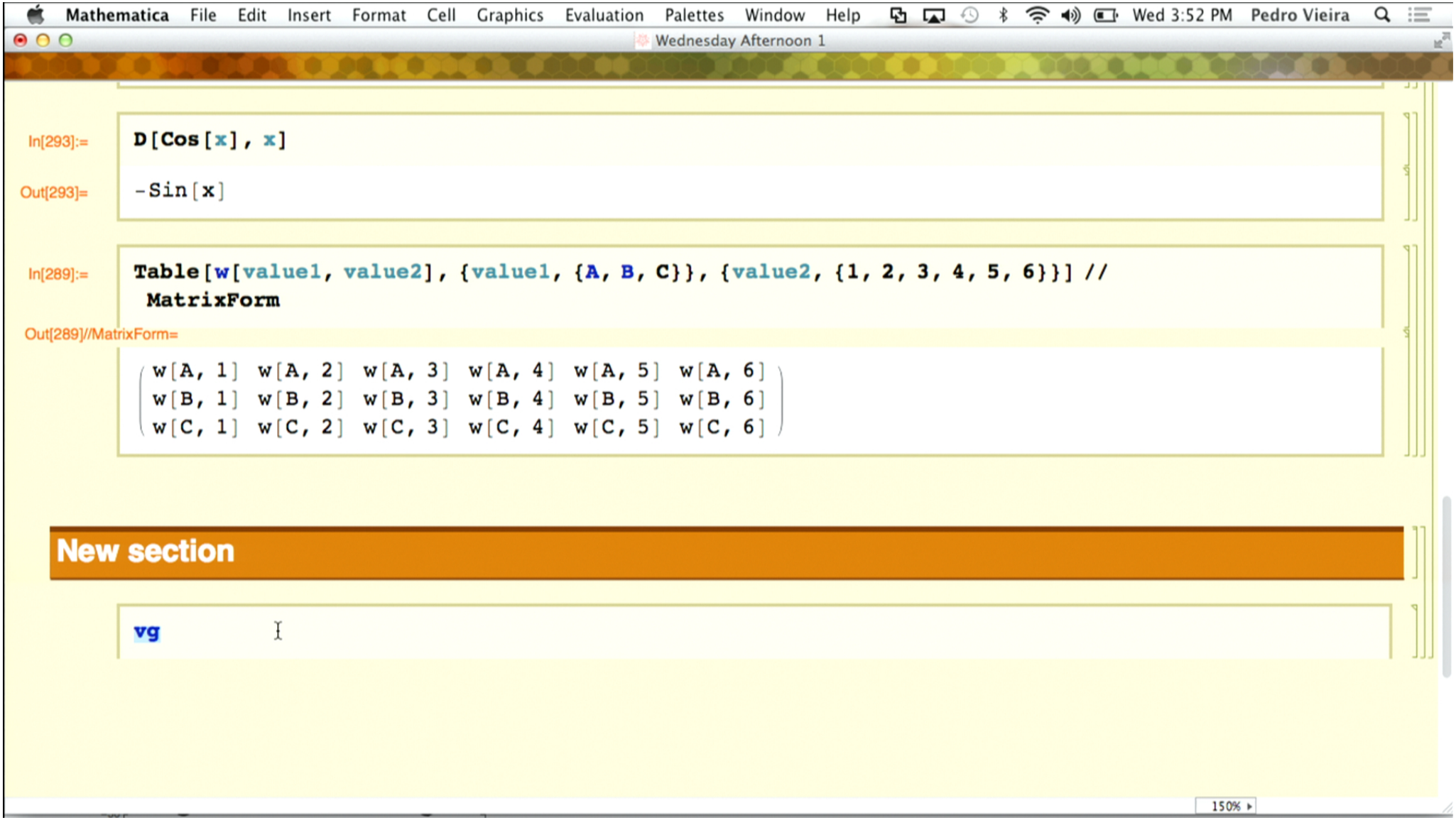

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:39 PM Pedro Vieira
Wednesday Afternoon 1
Out[255]= 10 138
In[256]:= k[x_, y_] /; x < y ∧ y > 0 := x y
In[258]:= k[98, 90]
Out[258]= k[98, 90]
150%

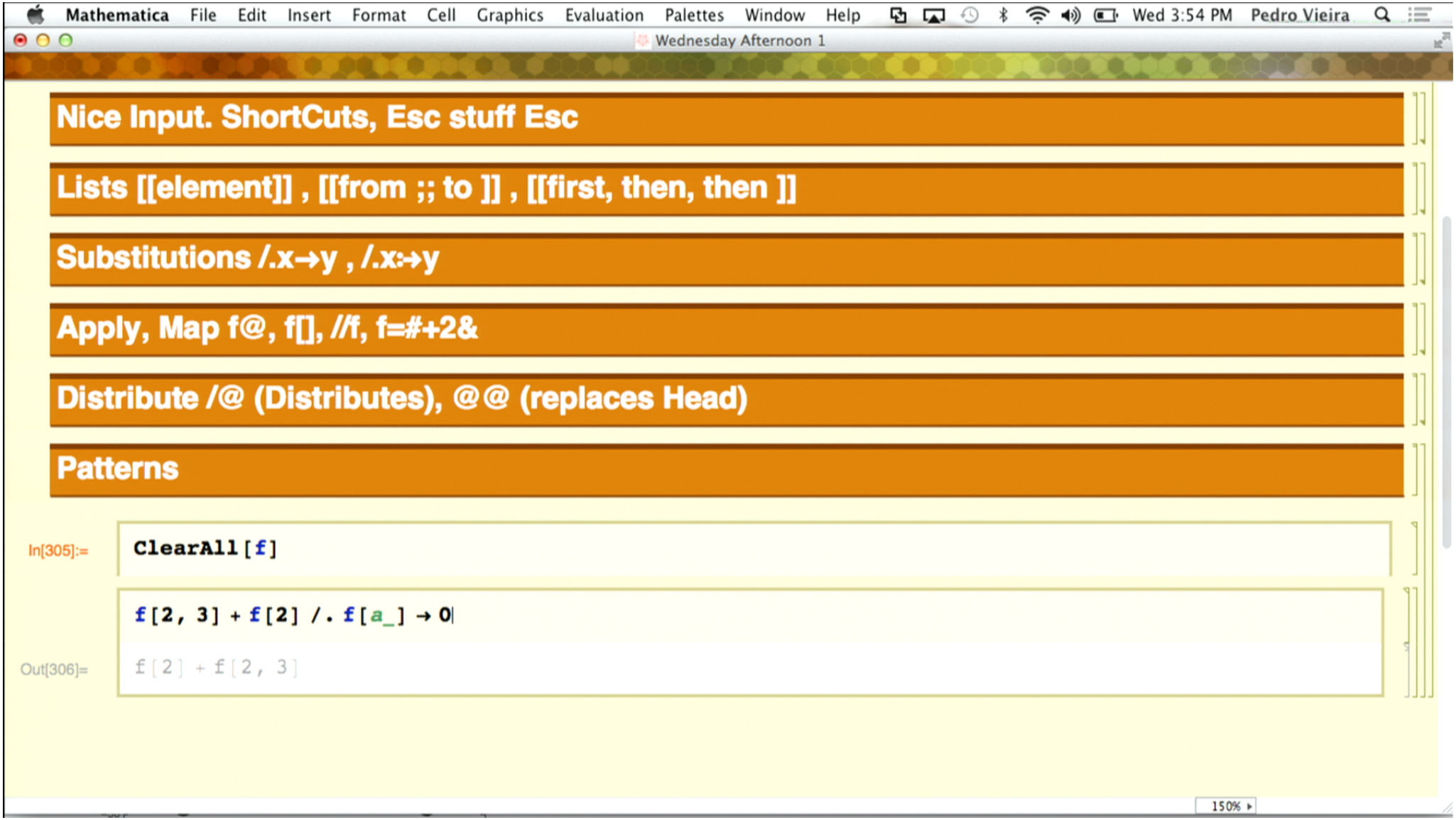

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:41 PM Pedro Vieira
Wednesday Afternoon 1
Basics of Mathematica
Shift + Enter
Equal signs =, :=, ==, ===
Nice Input
Lists [[element]] , [[from ;; to]] , [[first, then, then]]
Substitutions /.x→y , /.x:→y
Apply, Map f@, f[], //f
150%

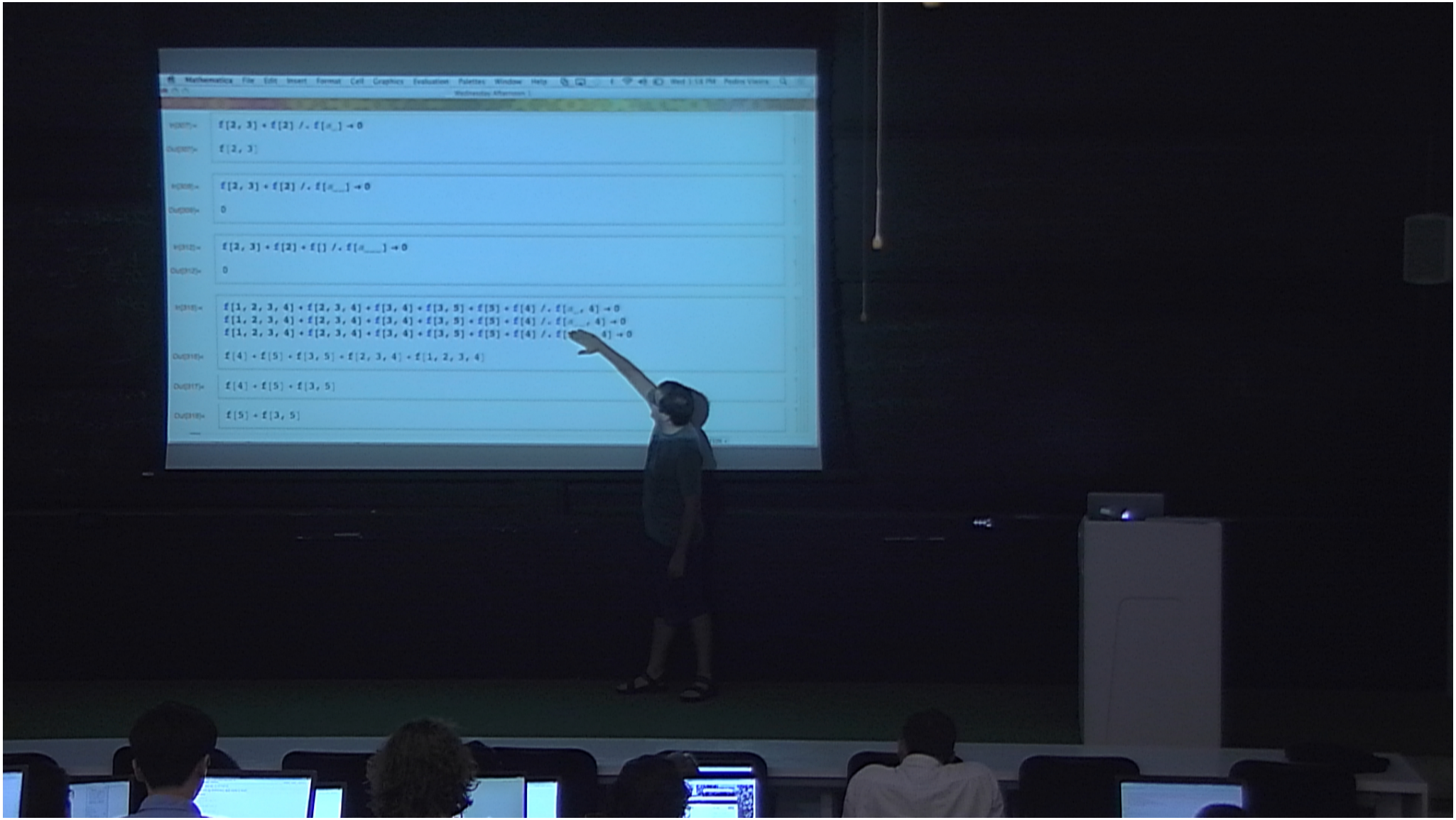

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:45 PM Pedro Vieira
Wednesday Afternoon 1
Substitutions /.x→y , /.x:→y
Apply, Map f@, f[], //f, f=#+2&
Distribute
In[274]:= u@{a, b, c, d}
Out[274]= u[{a, b, c, d}]
In[275]:= u /@ {a, b, c, d}
Out[275]= {u[a], u[b], u[c], u[d]}
#^2 &
150%

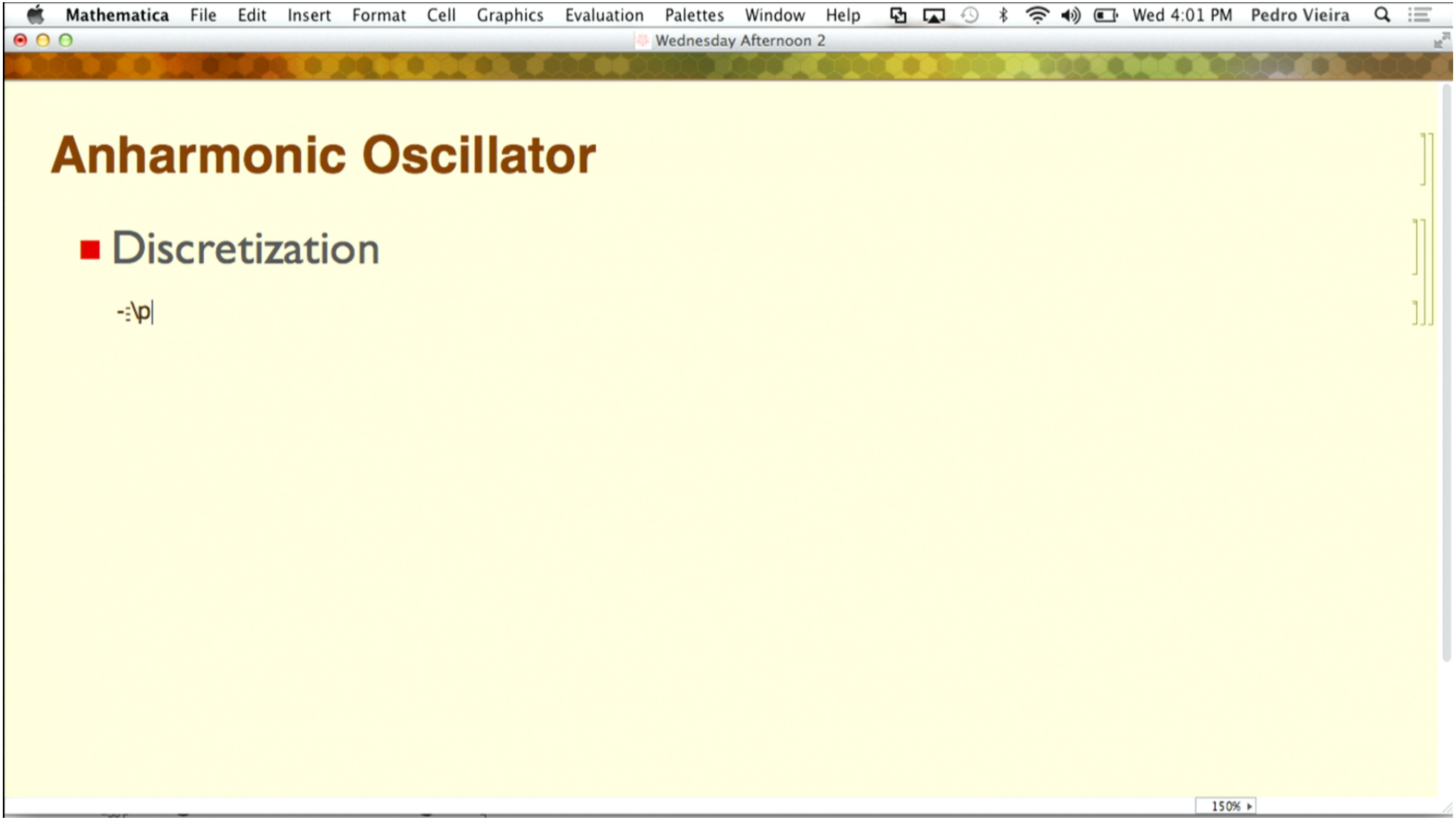

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:49 PM Pedro Vieira
Wednesday Afternoon 1
In[275]:= u /@ {a, b, c, d}
Out[275]= {u[a], u[b], u[c], u[d]}
In[284]:= ClearAll[x]
In[285]:= t[x_] = (x^2 + 1)/x;
In[286]:= t /@ {a, b, c, d}
Out[286]= {(1 + a^2)/a, (1 + b^2)/b, (1 + c^2)/c, (1 + d^2)/d}
In[279]:= ((#^2 + 1)/#) & /@ {a, b, c, d}
Out[279]= {(1 + a^2)/a, (1 + b^2)/b, (1 + c^2)/c, (1 + d^2)/d}
150%


Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:50 PM Pedro Vieira
Wednesday Afternoon 1
In[285]:= t[x_] = ;
x
In[286]:= t /@ {a, b, c, d}
Out[286]= {1 + a^2 / a, 1 + b^2 / b, 1 + c^2 / c, 1 + d^2 / d}
In[279]:= (#^2 + 1 / #) & /@ {a, b, c, d}
Out[279]= {1 + a^2 / a, 1 + b^2 / b, 1 + c^2 / c, 1 + d^2 / d}
In[287]:= Table[f[value1, value2], {value1, {A, B, C}}, {value2, {1, 2, 3, 4, 5, 6}}]
Out[287]= {{A, A^2, A^3, A^4, A^5, A^6}, {B, B^2, B^3, B^4, B^5, B^6}, {C, C^2, C^3, C^4, C^5, C^6}}
New section
150%


Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:52 PM Pedro Vieira
Wednesday Afternoon 1
In[293]:=
D[Cos[x], x]
Out[293]=
-Sin[x]
In[289]:=
Table[w[value1, value2], {value1, {A, B, C}}, {value2, {1, 2, 3, 4, 5, 6}}] //
MatrixForm
Out[289]//MatrixForm=
w[A, 1] w[A, 2] w[A, 3] w[A, 4] w[A, 5] w[A, 6]
w[B, 1] w[B, 2] w[B, 3] w[B, 4] w[B, 5] w[B, 6]
w[C, 1] w[C, 2] w[C, 3] w[C, 4] w[C, 5] w[C, 6]
New section
vg
150%


Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 3:54 PM Pedro Vieira
Wednesday Afternoon 1
Nice Input. ShortCuts, Esc stuff Esc
Lists [[element]] , [[from ;; to]] , [[first, then, then]]
Substitutions /.x→y , /.x:→y
Apply, Map f@, f[], //f, f=#+2&
Distribute /@ (Distributes), @@ (replaces Head)
Patterns
In[305]:=
ClearAll[f]
f[2, 3] + f[2] /. f[a_] → 0
Out[306]=
f[2] + f[2, 3]
150%


f[2, 3] + f[2] /. f[a_] → 0
f[2, 3]
f[3, 3] + f[2] /. f[a__] → 0
0
f[2, 3] + f[2] + f[] /. f[a___] → 0
0
f[1, 2, 3, 4] + f[2, 3, 4] + f[3, 4] + f[3, 5] + f[5] + f[4] /. f[a_, 4] → 0
f[1, 2, 3, 4] + f[2, 3, 4] + f[3, 4] + f[3, 5] + f[5] + f[4] /. f[a__, 4] → 0
f[4] + f[5] + f[3, 5] + f[2, 3, 4] + f[1, 2, 3, 4]
f[4] + f[5] + f[3, 5]
f[5] + f[3, 5]


Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help
Wed 4:01 PM Pedro Vieira
Wednesday Afternoon 2
Anharmonic Oscillator
Discretization
-:\p
150%

Anharmonic Oscillator

- Discretization

$$-\frac{1}{2}\partial^2\psi$$

Anharmonic Oscillator

- Discretization

$-\frac{1}{2}\partial^2\psi + V\psi == E\psi$ which becomes $-\frac{1}{2}\left(\frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{\delta x^2}\right) + V[$

Anharmonic Oscillator

Discretization

$-\frac{1}{2}\partial^2\psi + V\psi == E\psi$ which becomes

$-\frac{1}{2}\left(\frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{\delta x^2}\right) + V[x_i]\,\psi_i == E\,\psi_i$, i.e. we need to solve $M\cdot\vec{\psi} == \lambda\vec{\psi}$ with

$$V[x\_] = \frac{x^2}{2} + \frac{x^4}{24}$$

$$\delta$$

⋮

$$\left\{\{i\_, i\_\} \to V[\text{position}] + \frac{1}{\delta x^2}, \{i\_, j\_\} /; \text{Abs}[j - i] == 1 \to -\frac{1}{2\,\delta x^2}\right\}$$

150%

$-\frac{1}{2}\partial^2\psi + V\psi == E\psi$ which becomes

$-\frac{1}{2}\left(\frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{\delta x^2}\right) + V[x_i]\,\psi_i == E\,\psi_i$, i.e. we need to solve $M\cdot\vec{\psi} == \lambda\vec{\psi}$ with

$$V[x\_] = \left(-\frac{x^2}{2} + \frac{x^4}{24}\right);$$

$$\left\{\{i\_, i\_\} \to V[\text{position}] + \frac{1}{\delta x^2}, \{i\_, j\_\} /; \text{Abs}[j - i] == 1 \to -\frac{1}{2\,\delta x^2}\right\}$$

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 4:08 PM Pedro Vieira

Wednesday Afternoon 2

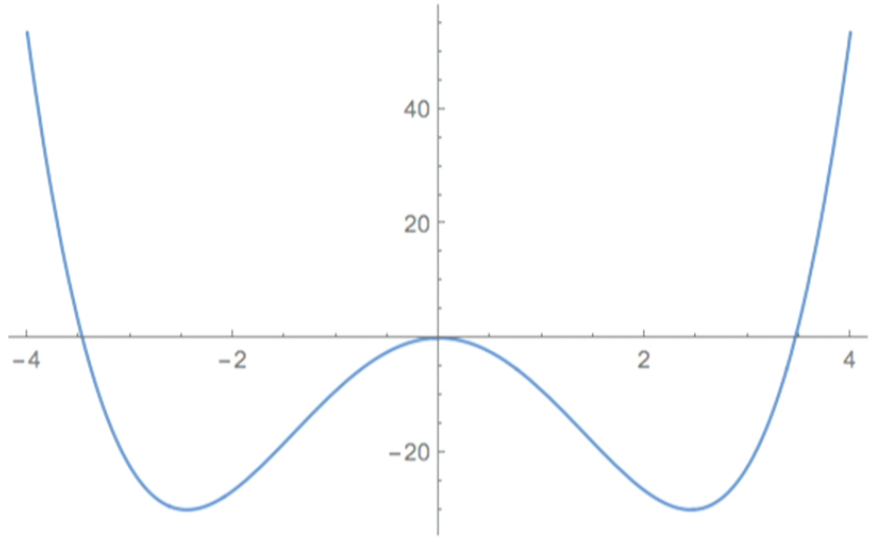
$-\frac{1}{2}\partial^2\psi + V\psi == E\psi$ which becomes

$-\frac{1}{2}\left(\frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{\delta x^2}\right) + V[x_i]\,\psi_i == E\,\psi_i$, i.e. we need to solve $M\cdot\vec{\psi} == \lambda\vec{\psi}$ with

In[325]:=
```
V[x_] = (-x^2/2 + x^4/24) 20;
```

In[326]:=
```
Plot[V[x], {x, -4, 4}]
```

Out[326]=



150%

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 4:10 PM Pedro Vieira

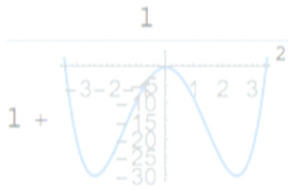
Wednesday Afternoon 2

$$2 \left(\frac{}{\delta x^2} \right)$$

In[329]:=
$$V[x\_] = \left(-\frac{x^2}{2} + \frac{x^4}{24} \right) 20;$$

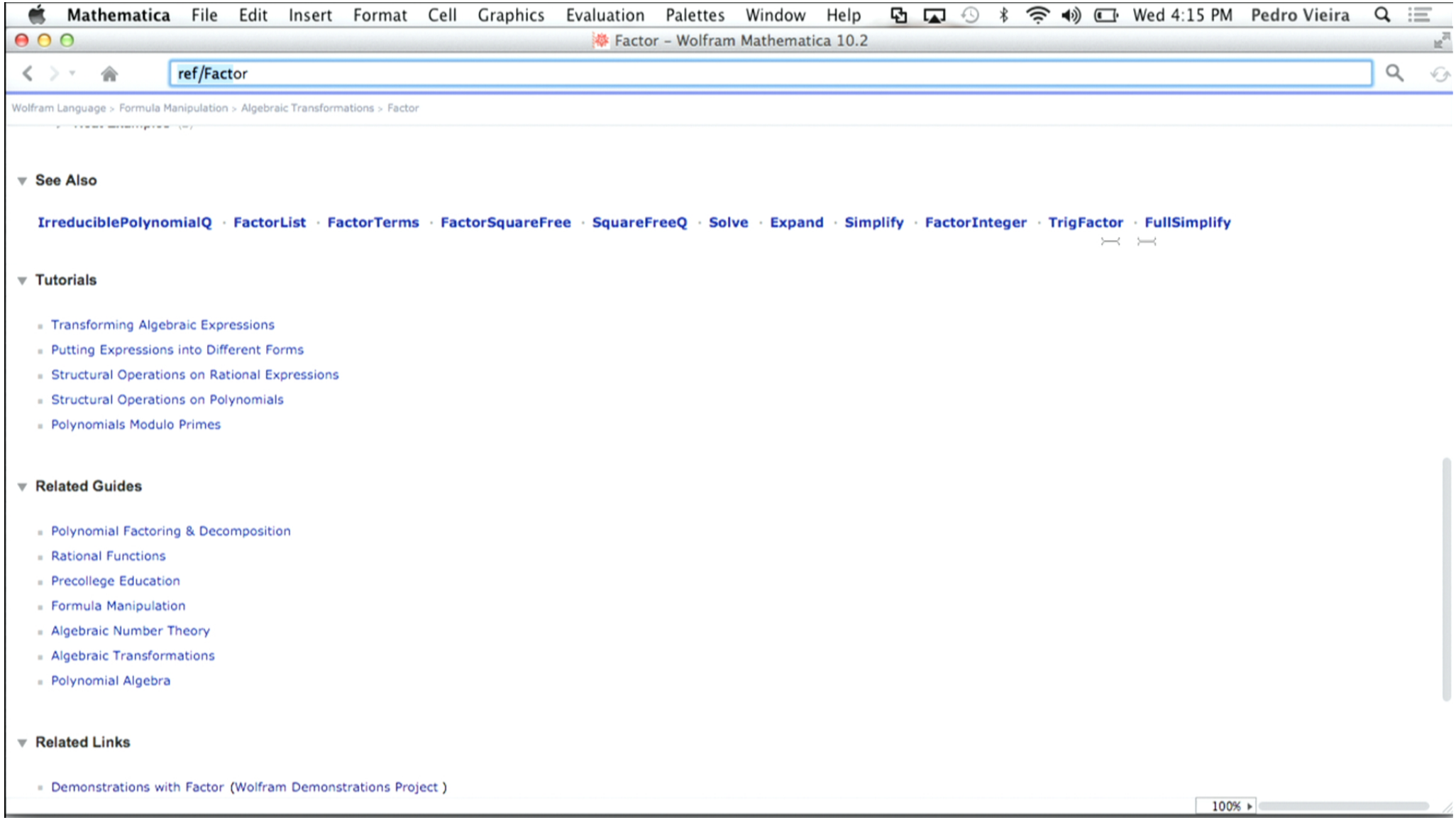
In[333]:=
$$\text{PlotV} = \text{Plot}[V[x], \{x, -3.5, 3.5\}];$$

Out[335]=
$$\frac{\square}{\text{PlotV}^2 + 1}$$



$$\left\{ \{i\_, i\_\} \to V[\text{position}] + \frac{1}{\delta x^2}, \{i\_, j\_\} /; \text{Abs}[j - i] == 1 \to -\frac{1}{2\,\delta x^2} \right\}$$

150%


Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 4:15 PM Pedro Vieira
Factor – Wolfram Mathematica 10.2
ref/Factor
Wolfram Language > Formula Manipulation > Algebraic Transformations > Factor
See Also
IrreduciblePolynomialQ · FactorList · FactorTerms · FactorSquareFree · SquareFreeQ · Solve · Expand · Simplify · FactorInteger · TrigFactor · FullSimplify
Tutorials
Transforming Algebraic Expressions
Putting Expressions into Different Forms
Structural Operations on Rational Expressions
Structural Operations on Polynomials
Polynomials Modulo Primes
Related Guides
Polynomial Factoring & Decomposition
Rational Functions
Precollege Education
Formula Manipulation
Algebraic Number Theory
Algebraic Transformations
Polynomial Algebra
Related Links
Demonstrations with Factor (Wolfram Demonstrations Project)
100%

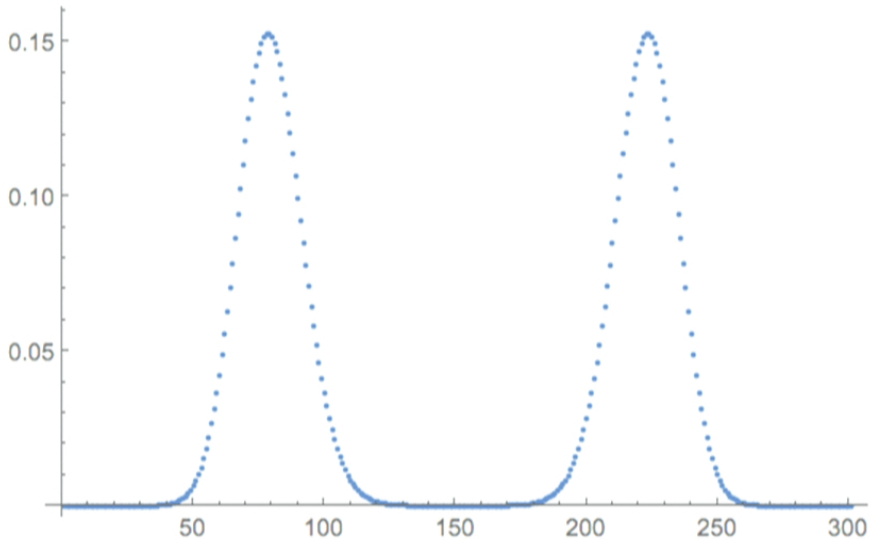
Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 4:27 PM Pedro Vieira

Wednesday Afternoon 2

Out[368]= {-26.882, -26.882, -20.8314, -20.8314, -15.091, -15.091, -9.72143, -9.72, -4.85438, -4.80738}

In[372]:=
```
es[[2, 1]] // ListPlot
```

Out[372]=



150%

Out[368]= {-26.882, -26.882, -20.8314, -20.8314, -15.091, -15.091, -9.72143, -9.72, -4.85438, -4.80738}

In[383]:=
```
? ListPlot
```

ListPlot[{y_1, y_2, ...}] plots points corresponding to a list of values, assumed to correspond to x coordinates 1, 2, ...
ListPlot[{{x_1, y_1}, {x_2, y_2}, ...}] plots a list of points with specified x and y coordinates.
ListPlot[{$list_1$, $list_2$, ...}] plots several lists of points. >>

In[381]:=
```
{Range[-L / 2, L / 2, δx], es[[2, 1]]}
```

Out[381]=
$$\left\{\left\{-5, -\frac{149}{30}, -\frac{74}{15}, -\frac{49}{10}, -\frac{73}{15}, -\frac{29}{6}, -\frac{24}{5}, -\frac{143}{30}, -\frac{71}{15}, -\frac{47}{10}, -\frac{14}{3}, -\frac{139}{30}, -\frac{23}{5}, -\frac{137}{30}, -\frac{68}{15}, -\frac{9}{2},\right.\right.$$
$$-\frac{67}{15}, -\frac{133}{30}, -\frac{22}{5}, -\frac{131}{30}, -\frac{13}{3}, -\frac{43}{10}, -\frac{64}{15}, -\frac{127}{30}, -\frac{21}{5}, -\frac{25}{6}, -\frac{62}{15}, -\frac{41}{10}, -\frac{61}{15}, -\frac{121}{30}, -4,$$
$$-\frac{119}{30}, -\frac{59}{15}, -\frac{39}{10}, -\frac{58}{15}, -\frac{23}{6}, -\frac{19}{5}, -\frac{113}{30}, -\frac{56}{15}, -\frac{37}{10}, -\frac{11}{3}, -\frac{109}{30}, -\frac{18}{5}, -\frac{107}{30}, -\frac{53}{15}, -\frac{7}{2},$$
$$-\frac{52}{15}, -\frac{103}{30}, -\frac{17}{5}, -\frac{101}{30}, -\frac{10}{3}, -\frac{33}{10}, -\frac{49}{15}, -\frac{97}{30}, -\frac{16}{5}, -\frac{19}{6}, -\frac{47}{15}, -\frac{31}{10}, -\frac{46}{15}, -\frac{91}{30}, -3,$$
$$-\frac{89}{30}, -\frac{44}{15}, -\frac{29}{10}, -\frac{43}{15}, -\frac{17}{6}, -\frac{14}{5}, -\frac{83}{30}, -\frac{41}{15}, -\frac{27}{10}, -\frac{8}{3}, -\frac{79}{30}, -\frac{13}{5}, -\frac{77}{30}, -\frac{38}{15}, -\frac{5}{2}, -\frac{37}{15},$$
$$-\frac{73}{30}, -\frac{12}{5}, -\frac{71}{30}, -\frac{7}{3}, -\frac{23}{10}, -\frac{34}{15}, -\frac{67}{30}, -\frac{11}{5}, -\frac{13}{6}, -\frac{32}{15}, -\frac{21}{10}, -\frac{31}{15}, -\frac{61}{30}, -2, -\frac{59}{30}, -\frac{29}{15},$$
$$\frac{19}{\quad} \quad \frac{28}{\quad} \quad \frac{11}{\quad} \quad 0 \quad \frac{53}{\quad} \quad \frac{26}{\quad} \quad \frac{17}{\quad} \quad 5 \quad \frac{49}{\quad} \quad 8 \quad \frac{47}{\quad} \quad \frac{23}{\quad} \quad 3 \quad \frac{22}{\quad} \quad \frac{43}{\quad} \quad 7$$

150%

Discretization

$-\frac{1}{2}\partial^2\psi + V\psi == E\psi$ which becomes

$-\frac{1}{2}\left(\frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{\delta x^2}\right) + V[x_i]\,\psi_i == E\,\psi_i$, i.e. we need to solve $M\cdot\vec{\psi} == \lambda\vec{\psi}$ with

```
V[x_] = (-x^2/2 + x^4/24) 5;

V[x_] = x^2/2;
```

In[402]:=
```
PlotV = Plot[V[x], {x, -3.5, 3.5}];
```

In[403]:=
```
n = 300;
L = 10;
δx = L / n;
```

In[406]:=
```
M = N@SparseArray[{{i_, i_} → V[-L/2 + (i - 1) δx] + 1/δx^2, {i_, j_} /; Abs[j - i] == 1 → -1/(2 δx^2)},
    {n + 1, n + 1}];
```

150%

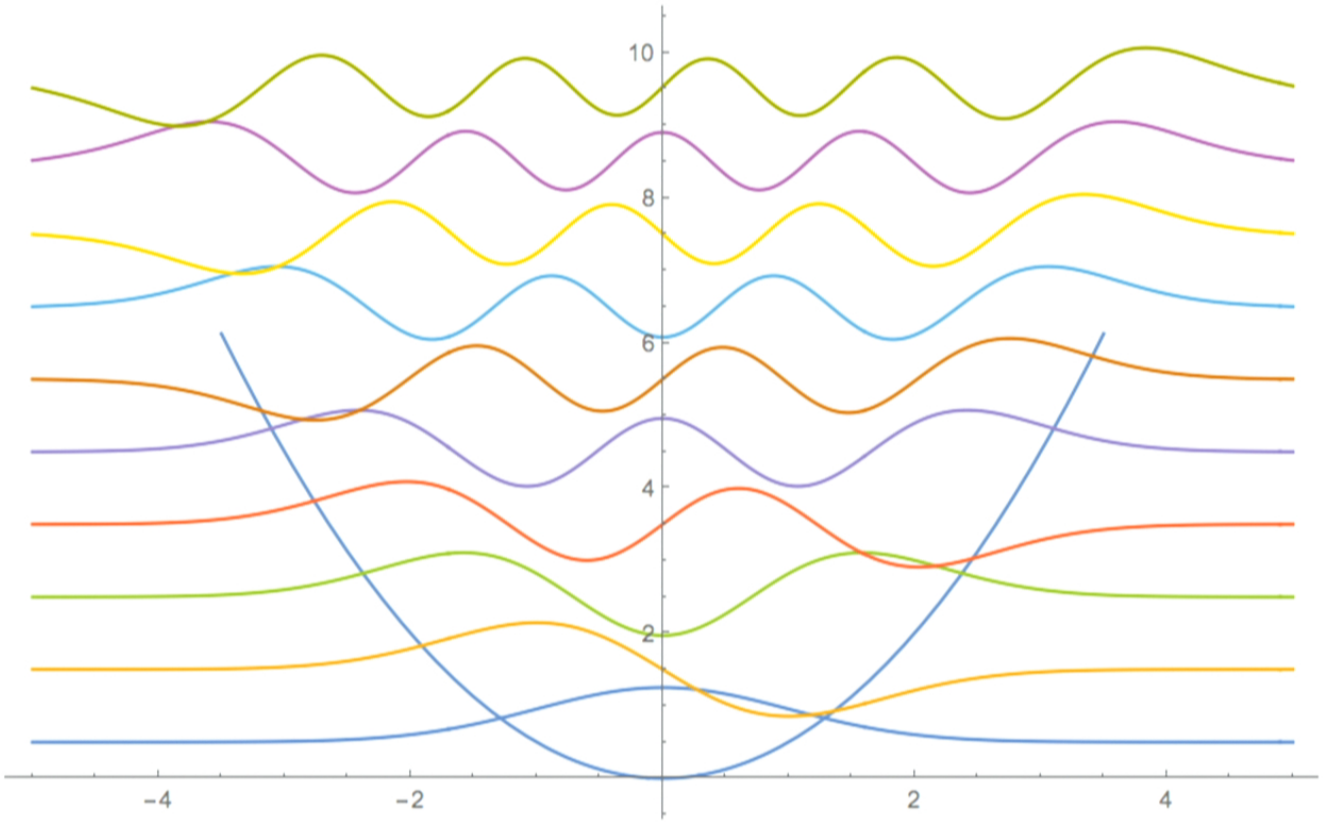
Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 4:42 PM Pedro Vieira

Wednesday Afternoon 2

In[426]:=

```
Show[PlotV, PlotWF, PlotRange → All]
```

Out[426]=



150%

Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 4:48 PM Pedro Vieira

Wednesday Afternoon 2

In[430]:=
```
n = 300;
L = 10;
δx = L / n;
```

In[433]:=
```
M = N@SparseArray[{{i_, i_} → V[-L/2 + (i - 1) δx] + 1/δx^2, {i_, j_} /; Abs[j - i] == 1 → -1/(2 δx^2)}, {n + 1, n + 1}];
```

In[434]:=
```
es = Eigensystem[M] // Transpose // Sort // #[[1 ;; 10]] & // Transpose // Quiet;
```

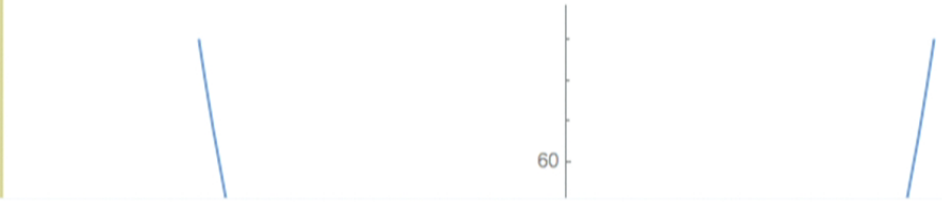
In[436]:=
```
es[[1]] // ListPlot
```

In[437]:=
```
es[[1]]
```

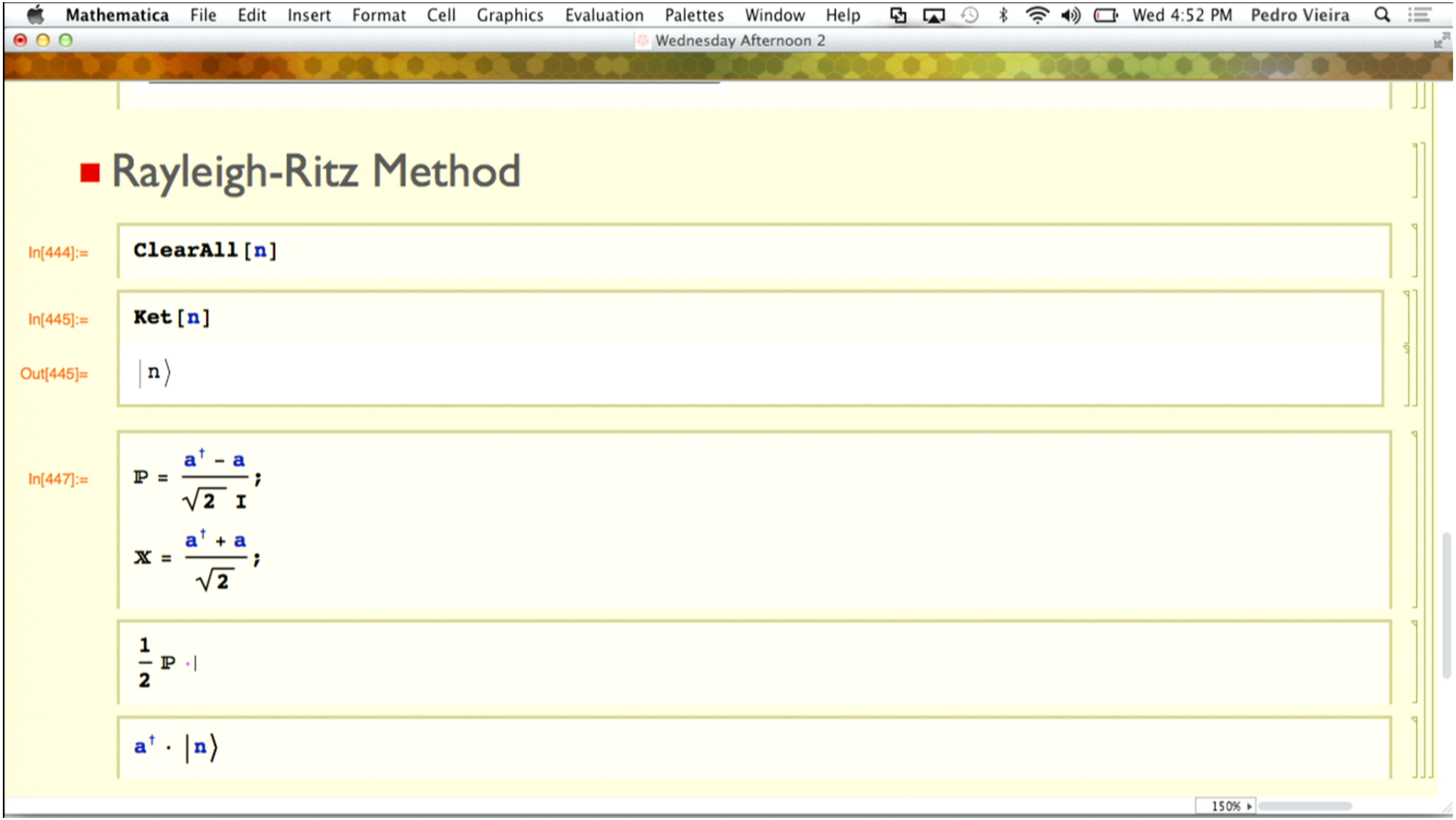
Out[437]=
```
{0.530115, 1.89937, 3.72625, 5.81863, 8.12373, 10.607, 13.2454, 16.0218, 18.9232, 21.9391}
```

In[438]:=
```
PlotWF = Table[{Range[-L / 2, L / 2, δx], es[[1, j]] + 1/Sqrt[δx] es[[2, j]]}^T, {j, 1, 10}] // ListPlot[#, Joined → True] &;
```

In[439]:=
```
Show[PlotV, PlotWF, PlotRange → All]
```



125%


Mathematica File Edit Insert Format Cell Graphics Evaluation Palettes Window Help Wed 4:52 PM Pedro Vieira
Wednesday Afternoon 2
Rayleigh-Ritz Method
In[444]:= ClearAll[n]
In[445]:= Ket[n]
Out[445]= |n⟩
In[447]:= ℙ = (a† - a)/(√2 ⅈ);
𝕏 = (a† + a)/√2;
1/2 ℙ ·|
a† · |n⟩
150%

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Wednesday Afternoon 2

$$\frac{\mathbf{I}}{\sqrt{2}},$$

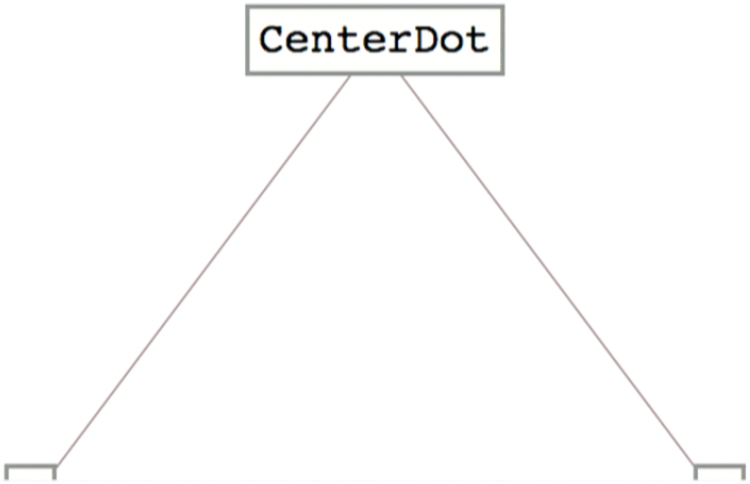
$$\mathbf{X} = \frac{\mathbf{a}^{\dagger} + \mathbf{a}}{\sqrt{2}};$$

In[451]:=
```
? CenterDot
```

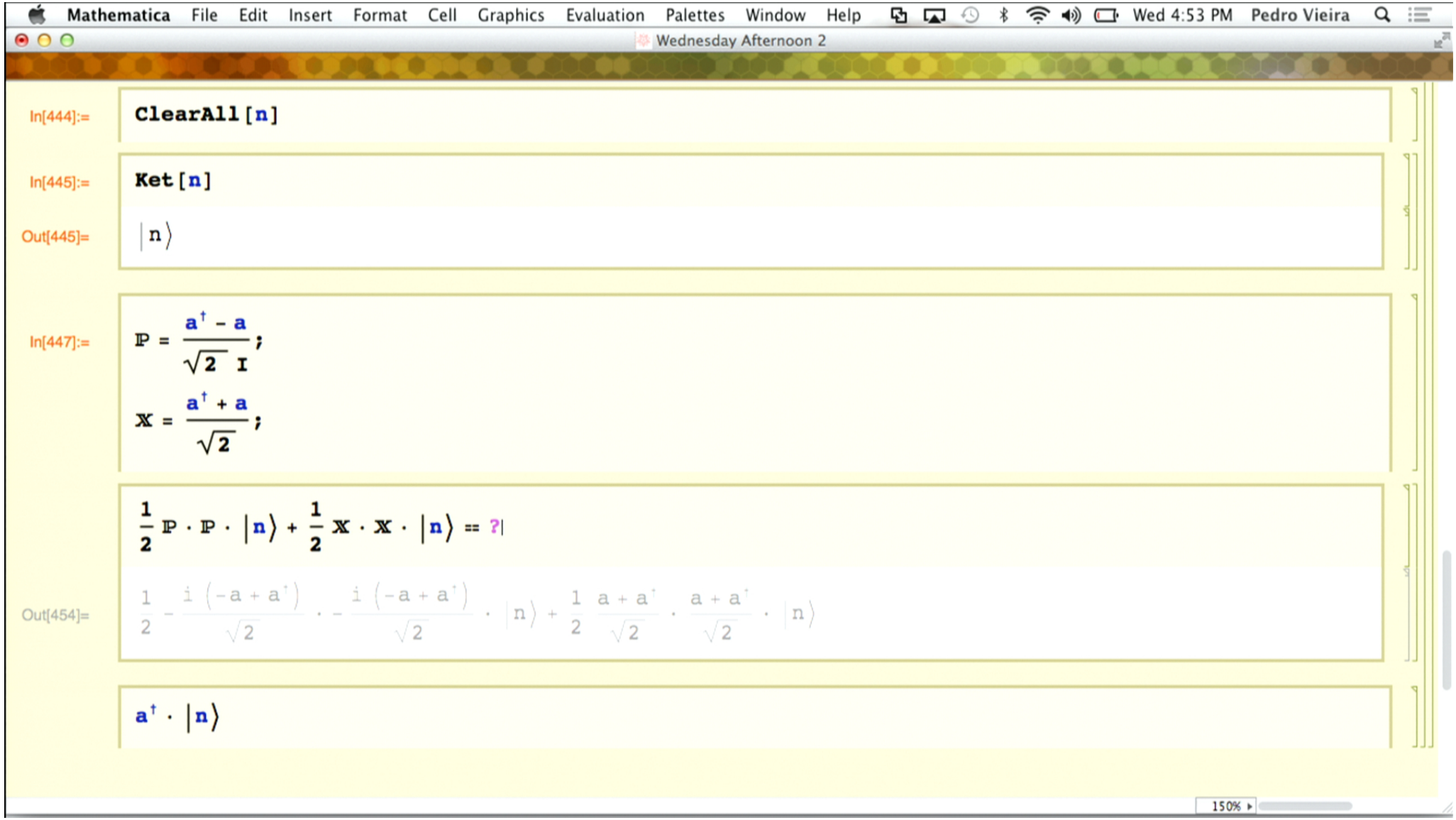
CenterDot[x, y, ...] displays as $x \cdot y \cdot \ldots$ >>

In[450]:=
```
a · b // TreeForm
```

Out[450]//TreeForm=



150%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Wednesday Afternoon 2
In[444]:= ClearAll[n]
In[445]:= Ket[n]
Out[445]= |n⟩
In[447]:= P = (a† - a)/(√2 I);
X = (a† + a)/√2;
1/2 P · P · |n⟩ + 1/2 X · X · |n⟩ == ?
Out[454]= 1/2 - i(-a + a†)/√2 · - i(-a + a†)/√2 · |n⟩ + 1/2 a + a†/√2 · a + a†/√2 · |n⟩
a† · |n⟩
150%

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In[546]:=
```
Hmatrix // Eigenvalues // Sort // 2 Take[#, 6] & // TableForm
```

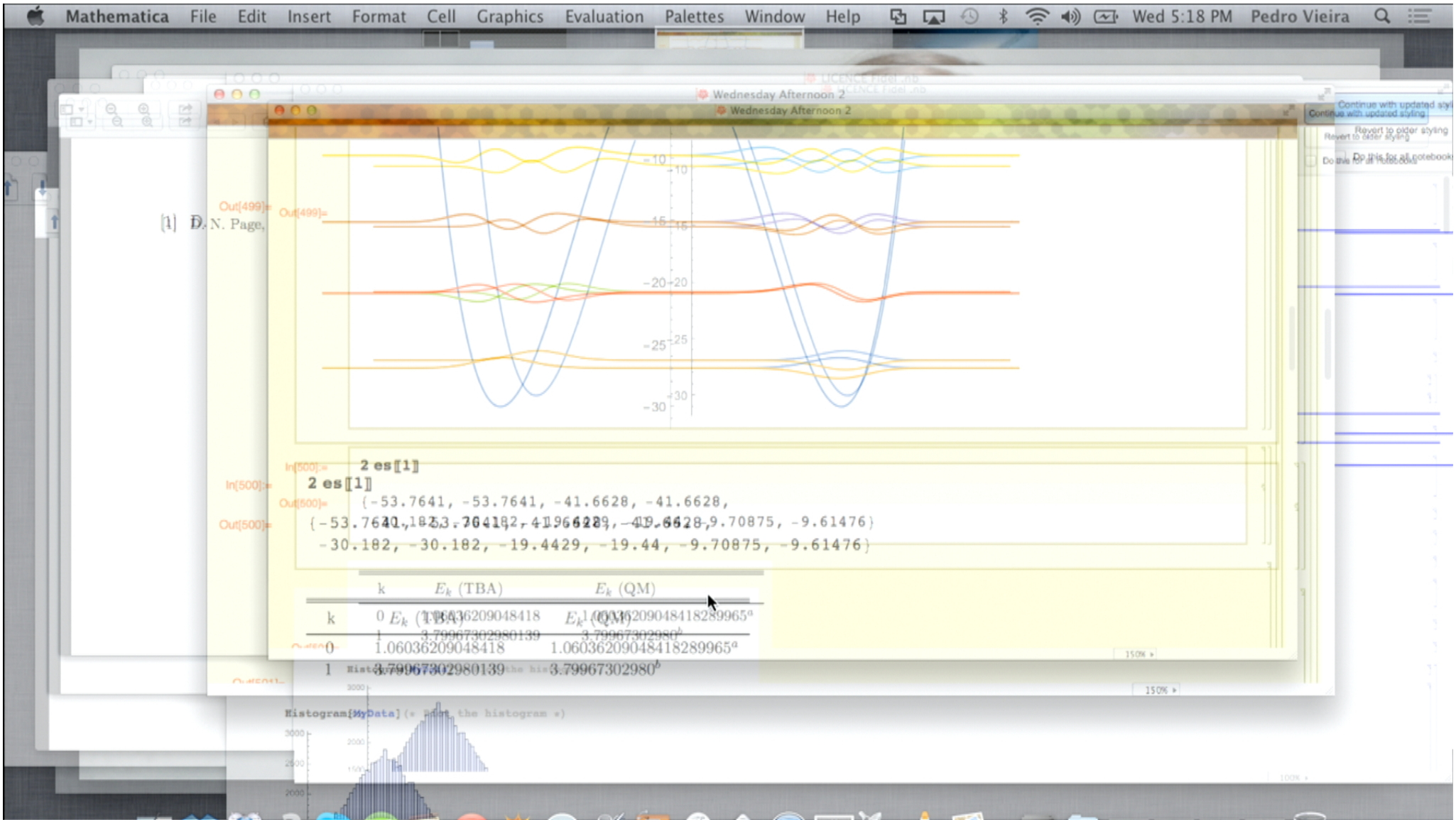
Out[546]//TableForm=

```
1.06036209048420504060514115478
3.79967302980165180043426845121
7.45569793798800583738540574770
11.64474551141137309572066379 92
16.26182601908079260314895855 25
21.23837291876952939318454500 43
```

Out[543]=

k	E_k (TBA)	E_k (QM)
0	1.06036209048418	$1.060362090484182899 65^a$
1	3.79967302980139	3.79967302980^b
2	7.45569793798672	$7.455697937986738392 16^a$
3	11.64474551137815	11.6447455114^b
4	16.26182601885024	$16.261826018850225937 89^a$
5	21.23837291823595	21.2383729182^b

150%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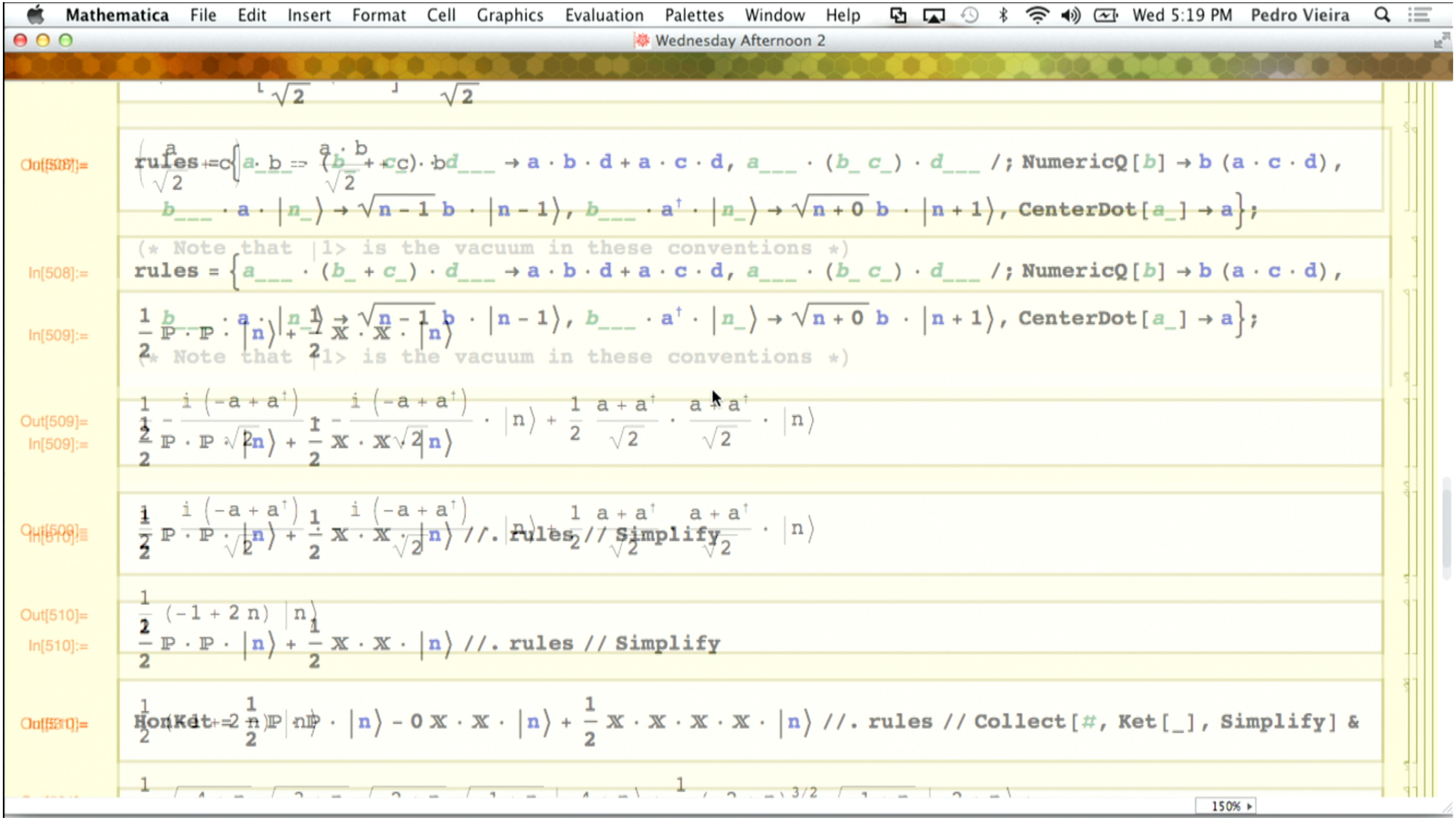
Wednesday Afternoon 2
Wednesday Afternoon 2
Out[499]=
[1] D. N. Page,
In[500]:= 2 es[[1]]
2 es[[1]]
Out[500]= {-53.7641, -53.7641, -41.6628, -41.6628,
-30.182, -30.182, -19.4429, -19.44, -9.70875, -9.61476}
k E_k (TBA) E_k (QM)
0 1.06036209048418 1.06036209048418289965[a]
1 3.79967302980139 3.79967302980[b]
Histogram[MyData]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Wednesday Afternoon 2
rules = {a___ · (b_ + c_) · d___ :> a · b · d + a · c · d, a___ · (b_ c_) · d___ /; NumericQ[b] :> b (a · c · d),
b___ · a · |n_⟩ :> √(n - 1) b · |n - 1⟩, b___ · a† · |n_⟩ :> √(n + 0) b · |n + 1⟩, CenterDot[a_] :> a};
(* Note that |1> is the vacuum in these conventions *)
In[508]:=
In[509]:=
Out[509]=
In[509]:=
Out[510]=
In[510]:=
rules // Simplify
150%

Anharmonic Oscillator

Discretization

$-\frac{1}{2}\partial^2\psi + V\psi == E\psi$ which becomes

$-\frac{1}{2}\left(\frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{\delta x^2}\right) + V[x_i]\,\psi_i == E\,\psi_i$, i.e. we need to solve $M\cdot\vec{\psi} == \lambda\vec{\psi}$ with

In[487]:=
$$V[x\_] = \frac{x^4}{2};$$
$$V[x\_] = \left(-\frac{x^2}{2} + \frac{x^4}{24}\right) 20;$$

In[489]:=
```
PlotV = Plot[V[x], {x, -3.5, 3.5}];
```

In[490]:=
```
n = 300;
L = 10;
δx = L / n;
```

150%

Out[504]= $|n\rangle$

In[505]:=
$$\mathbb{P} = \frac{a^\dagger - a}{\sqrt{2}\ \mathbb{I}};$$
$$\mathbb{X} = \frac{a^\dagger + a}{\sqrt{2}};$$

In[507]:=
$$\text{CenterDot}\left[\frac{a}{\sqrt{2}} + c,\ b\right] == \frac{1}{\sqrt{2}}\, a \cdot b + c \cdot b$$

Out[507]=
$$\left(\frac{a}{\sqrt{2}} + c\right) \cdot b == \frac{a \cdot b}{\sqrt{2}} + c \cdot b$$

In[508]:=
```
rules = {a___ · (b_ + c_) · d___ → a · b · d + a · c · d, a___ · (b_ c_) · d___ /; NumericQ[b] → b (a · c · d),
  b___ · a · |n_⟩ → √(n - 1) b · |n - 1⟩, b___ · a† · |n_⟩ → √(n + 0) b · |n + 1⟩, CenterDot[a_] → a};
|(* Note that |1> is the vacuum in these conventions *)
```

In[509]:=
$$\frac{1}{}\ \mathbb{P} \cdot \mathbb{P} \cdot |n\rangle + \frac{1}{}\ \mathbb{X} \cdot \mathbb{X} \cdot |n\rangle$$

150%