Title: Computer Algebra for Theoretical Physics (II)

Date: Oct 24, 2017 10:00 AM

URL: http://pirsa.org/17100083

Abstract: <p>Generally speaking, physicists still experience that computing with paper and pencil is in most cases simpler than computing with a Computer Algebra System. Although that is true in some cases, the working paradigm is changing: developments in CAS, and particularly recent ones in the Maple system, have resulted in the implementation of most of the mathematical objects and mathematics used in theoretical physics computations, and have dramatically approximated the notation used in the computer to the one used with paper and pencil, diminishing the learning gap and computer-syntax distraction to a strict minimum. In this talk, the Physics project at Maplesoft will be presented and the resulting Physics package will be illustrated through simple problems in classical field theory, quantum mechanics and general relativity, and through tackling the computations of some recent Physical Review papers in those areas. In addition to the 10:00 am lecture (taking place in Alice), there will be an afternoon hands-on workshop taking place in the Time Room.</p>

# Computer Algebra in Theoretical Physics

***Edgardo S. Cheb-Terrab***
***Physics, Differential Equations and Mathematical Functions, Maplesoft***

## Abstract:

*Generally speaking, physicists still experience that computing with paper and pencil is in most cases simpler than computing with a Computer Algebra System. Although that is true in some cases, the working paradigm is changing: developments in CAS, and particularly recent ones in the Maple system, have resulted in the implementation of most of the mathematical objects and mathematics used in theoretical physics computations, and have dramatically approximated the notation used in the computer to the one used with paper and pencil, diminishing the learning gap and computer-syntax distraction to a strict minimum.*

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# ... and why computer algebra?

***We can concentrate more on the ideas instead of on the algebraic manipulations***

***We can extend results with ease***

***We can explore the mathematics surrounding a problem***

***We can share results in a reproducible way***

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# Representation issues that were preventing the use of computer algebra in Physics

## Notation and related mathematical methods that were missing:

*coordinate free representations for vectors and vectorial differential operators,*
*covariant tensors distinguished from contravariant tensors, sum rule for tensor contracted (repeated) indices*
*functional differentiation, spacetime and covariant differential operators*
*Bras, Kets, projectors and all related to Dirac's notation in Quantum Mechanics*

## Inert representations of operations, mathematical functions, and related typesetting were missing:

*inert versus active representations for mathematical operations*

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## Inert representations of operations, mathematical functions, and related typesetting were missing:

*inert versus active representations for mathematical operations*
*hand-like style for entering computations, and computationally active output with textbook-like notation*

## Key elements of the computational domain of theoretical physics were missing:

*product and differentiation handling commutative, anticommutative and noncommutative variables and functions*
*ability to set custom-defined algebra rules (commutator, anticommutator and bracket rules, etc.)*
*ability to distinguisn between generic, unitary and Hermitian quantum operators*

>

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# The Maple computer algebra environment

- In the presentation that follows we use the Maple worksheet mode, where input lines are identified by a prompt, as in:
- We communicate with the computer entering our computation typing in this input line. The output is the result of our computation and automatically gets an equation number than we can later refer to. We use inert and active forms

>

- To refer to an equation, you enter the equation label by pressing Command + L, then typing the equation number as you see it

> ??

>

# Classical Mechanics

# Quantum mechanics

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- To refer to an equation, you enter the equation label by pressing Command + L, then typing the equation number as you see it

> $(\%int = int)(\cos(x), x)$

$$\int \cos(x)\, dx = \sin(x) \qquad (1)$$

> (1)

$$\int \cos(x)\, dx = \sin(x) \qquad (2)$$

>

# Classical Mechanics

## Inertia tensor for a triatomic molecule

**Problem:** Determine the Inertia tensor of a triatomic molecule that has the form of an isosceles triangle with two masses $m_1$ in the extremes of the base and mass $m_2$ in the third vertex. The distance between the two masses $m_1$ is equal to $a$, and the height of the triangle is equal to $h$.

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> (1)

$$\int \cos(x)\, dx = \sin(x) \qquad (2)$$

>

# Classical Mechanics

## Inertia tensor for a triatomic molecule

**Problem:** Determine the Inertia tensor of a triatomic molecule that has the form of an isosceles triangle with two masses $m_1$ in the extremes of the base and mass $m_2$ in the third vertex. The distance between the two masses $m_1$ is equal to $a$, and the height of the triangle is equal to $h$.

### *Solution*

> *restart*; *with*(*Physics*, *KroneckerDelta*) : *with*(*Physics*[*Vectors*]) :

The general formula

> $InertiaTensor := \%sum\left(m[k]\left(Norm(r\_[k])^2 KroneckerDelta[i,j] - Component(r\_[k], i)\, Component(r\_[k], j)\right), k = 1 .. N\right);$

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## Solution

> $restart; with(Physics, KroneckerDelta) : with(Physics[Vectors]) :$

The general formula

> $InertiaTensor := \%sum\left(m[k]\ \left(Norm(r\_[k])^2\ KroneckerDelta[i, j] - Component(r\_[k], i)\ Component(r\_[k], j)\right), k = 1 .. N\right);$

There are 3 particles

> $N := 3$

Create an indexing function

> $IT := unapply(InertiaTensor, i, j)$

The inert tensor matrix

> $IT\_Matrix := Matrix(3, IT)$

Choose a system of reference (not at the center of mass). The vectors $\vec{r}_k$ are related to $\vec{R}_k$ and $\vec{R}_{CM}$ by

> $position := r\_[k] = R\_[k] - R\_[CM];$

Choose the origin at the middle of the segment connecting the two atoms of equal mass

> $R\_[1] := -\frac{a}{2}\ \_i;$

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**Solution**

```
> restart; with(Physics, KroneckerDelta) : with(Physics[Vectors]) :
```

The general formula

```
> InertiaTensor := %sum(m[k] (Norm(r_[k]))^2 KroneckerDelta[i, j] - Component(r_[k], i) Component(r_[k], j)), k = 1 .. N);
```

There are 3 particles

```
> N := 3
```

Create an indexing function

```
> IT := unapply(InertiaTensor, i, j)
```

The inert tensor matrix

```
> IT_Matrix := Matrix(3, IT)
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Choose a system of reference (not at the center of mass). The vectors $\vec{r}_k$ are related to $\vec{R}_k$ and $\vec{R}_{CM}$ by

```
> position := r_[k] = R_[k] - R_[CM];
```

Choose the origin at the middle of the segment connecting the two atoms of equal mass

> $R\_[1] := -\frac{a}{2}\_i;$

> $R\_[2] := h\_k$

> $R\_[3] := \frac{a}{2}\_i$

Two masses are equal

> $m_3 := 2 \cdot m[1]$

The "*center of mass*"

```
> R_[CM] := Sum(m[j] R_[j], j = 1 .. N) / Sum(m[j], j = 1 .. N);
```

> $\vec{R}_{CM} := value(\vec{R}_{CM})$

The positions of the three particles viewed from the center of mass

```
> seq(eval(position, k = j), j = 1 .. N)
```

The abstract IT_Matrix at these values of the vectors $\vec{r}_k$

```
> IT_answer := simplify(eval(value(IT_Matrix), [??]))
>
```

# Quantum mechanics

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## Solution

> restart; with(Physics, KroneckerDelta) : with(Physics[Vectors]) :

The general formula

> InertiaTensor := %sum(m[k] (Norm(r_[k])^2 KroneckerDelta[i,j] - Component(r_[k], i) Component(r_[k], j)), k = 1 .. N);

$$InertiaTensor := \sum_{k=1}^{N} m_k \left( \|\vec{r}_k\|^2 \delta_{i,j} - (\vec{r}_k)_i (\vec{r}_k)_j \right) \quad (3)$$

There are 3 particles

> N := 3

Create an indexing function

> IT := unapply(InertiaTensor, i, j)

The inert tensor matrix

> IT_Matrix := Matrix(3, IT)

Choose a system of reference (not at the center of mass). The vectors $\vec{r}_k$ are related to $\vec{R}_k$ and $\vec{R}_{CM}$ by

> position := r_[k] = R_[k] - R_[CM];

Choose the origin at the middle of the segment connecting the two atoms of equal mass

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$$IT := (i, j) \mapsto \sum_{k=1} m_k \left( \|\vec{r}_k\|^2 \delta_{i,j} - (\vec{r}_k)_i (\vec{r}_k)_j \right) \quad (5)$$

The inert tensor matrix

> $IT\_Matrix := Matrix(3, IT)$

$$IT\_Matrix := \begin{bmatrix} \sum_{k=1}^{3} m_k \left( \|\vec{r}_k\|^2 - (\vec{r}_k)_1^{\,2} \right) & \sum_{k=1}^{3} \left( -m_k (\vec{r}_k)_1 (\vec{r}_k)_2 \right) & \sum_{k=1}^{3} \left( -m_k (\vec{r}_k)_1 (\vec{r}_k)_3 \right) \\ \sum_{k=1}^{3} \left( -m_k (\vec{r}_k)_1 (\vec{r}_k)_2 \right) & \sum_{k=1}^{3} m_k \left( \|\vec{r}_k\|^2 - (\vec{r}_k)_2^{\,2} \right) & \sum_{k=1}^{3} \left( -m_k (\vec{r}_k)_2 (\vec{r}_k)_3 \right) \\ \sum_{k=1}^{3} \left( -m_k (\vec{r}_k)_1 (\vec{r}_k)_3 \right) & \sum_{k=1}^{3} \left( -m_k (\vec{r}_k)_2 (\vec{r}_k)_3 \right) & \sum_{k=1}^{3} m_k \left( \|\vec{r}_k\|^2 - (\vec{r}_k)_3^{\,2} \right) \end{bmatrix} \quad (6)$$

Choose a system of reference (not at the center of mass). The vectors $\vec{r}_k$ are related to $\vec{R}_k$ and $\vec{R}_{CM}$ by

> $position := r\_[k] = R\_[k] - R\_[CM];$

$$position := \vec{r}_k = \vec{R}_k - \vec{R}_{CM} \quad (7)$$

Choose the origin at the middle of the segment connecting the two atoms of equal mass

> $R\_[1] := -\frac{a}{2}\_i;$

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$$IT\_Matrix := \begin{bmatrix} \sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_1 \left(\vec{r}_k\right)_2\right) & \sum_{k=1}^{3} m_k \left(\left\|\vec{r}_k\right\|^2 - \left(\vec{r}_k\right)_2^{\,2}\right) & \sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_2 \left(\vec{r}_k\right)_3\right) \\ \sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_1 \left(\vec{r}_k\right)_3\right) & \sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_2 \left(\vec{r}_k\right)_3\right) & \sum_{k=1}^{3} m_k \left(\left\|\vec{r}_k\right\|^2 - \left(\vec{r}_k\right)_3^{\,2}\right) \end{bmatrix} \quad (6)$$

Choose a system of reference (not at the center of mass). The vectors $\vec{r}_k$ are related to $\vec{R}_k$ and $\vec{R}_{CM}$ by

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$$position := \vec{r}_k = \vec{R}_k - \vec{R}_{CM} \quad (7)$$

Choose the origin at the middle of the segment connecting the two atoms of equal mass

> $R\_[1] := -\frac{a}{2}\_i;$

> $R\_[2] := h\_k$

> $R\_[3] := \frac{a}{2}\_i$

Two masses are equal

> $m_3 := 2 \cdot m[1]$

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> $R\_[2] := h\ \_k$

$$\vec{R}_2 := h\ \hat{k} \tag{9}$$

> $R\_[3] := \frac{a}{2}\ \_i$

$$\vec{R}_3 := \frac{a\ \hat{i}}{2} \tag{10}$$

Two masses are equal

> $m_3 := m[1]$

$$m_3 := m_1 \tag{11}$$

The "*center of mass*"

> $R\_[CM] := Sum(m[j]\ R\_[j], j = 1\ ..\ N)\ /\ Sum(m[j], j = 1\ ..\ N);$

$$\vec{R}_{CM} := \frac{\sum_{j=1}^{3} m_j\ \vec{R}_j}{\sum_{j=1}^{3} m_j} \tag{12}$$

> $\vec{R}_{CM} := value(\vec{R}_{CM})$

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$$IT\_answer := \begin{bmatrix} 0 & \frac{8\,a^2\,m_1 + 3\,m_2\,(a^2 + 4\,h^2)\,m_1}{12\,m_1 + 4\,m_2} & 0 \\ \frac{m_1\,a\,m_2\,h}{6\,m_1 + 2\,m_2} & 0 & \frac{m_1\,a^2\,(8\,m_1 + 3\,m_2)}{12\,m_1 + 4\,m_2} \end{bmatrix} \quad (7)$$

>

# Quantum mechanics

## The quantum operator components of $\vec{L}$ satisfy $[L_j, L_k]_- = i\,\epsilon_{j,k,m}\,L_m$

> *restart; with(Physics) : interface(imaginaryunit = i) :*

> *Setup(spaceindices = lowercaselatin, metric = Euclidean, automaticsimplification = true)*

Define $L$, $r$ and $p$ as tensors of the 3-D Euclidean space embedded in

> *Define(L, r, p)*

Now set $L$, $p$, $r$ as quantum operators and the related **Commutator** rules for the algebra in tensor notation

> *Setup(quantumoperators = {L, p, r},*

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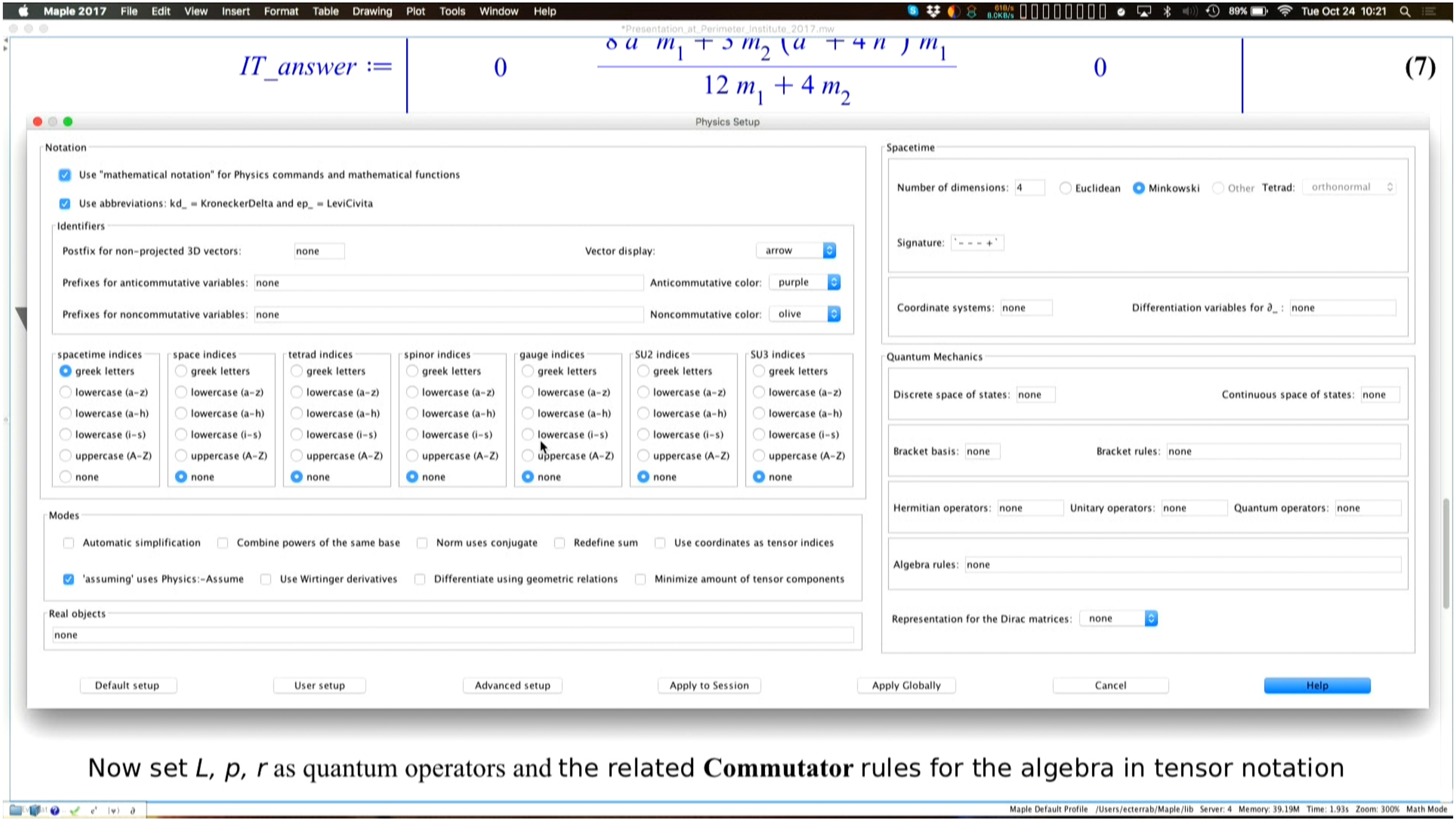
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Tue Oct 24 10:21
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IT_answer :=
0
12 m1 + 4 m2
0
(7)
Physics Setup
Notation
Use "mathematical notation" for Physics commands and mathematical functions
Use abbreviations: kd_ = KroneckerDelta and ep_ = LeviCivita
Identifiers
Postfix for non-projected 3D vectors: none
Vector display: arrow
Prefixes for anticommutative variables: none
Anticommutative color: purple
Prefixes for noncommutative variables: none
Noncommutative color: olive
spacetime indices
space indices
tetrad indices
spinor indices
gauge indices
SU2 indices
SU3 indices
greek letters
lowercase (a-z)
lowercase (a-h)
lowercase (i-s)
uppercase (A-Z)
none
Modes
Automatic simplification
Combine powers of the same base
Norm uses conjugate
Redefine sum
Use coordinates as tensor indices
'assuming' uses Physics:-Assume
Use Wirtinger derivatives
Differentiate using geometric relations
Minimize amount of tensor components
Real objects
none
Spacetime
Number of dimensions: 4
Euclidean
Minkowski
Other
Tetrad: orthonormal
Signature: `- - - +`
Coordinate systems: none
Differentiation variables for ∂_ : none
Quantum Mechanics
Discrete space of states: none
Continuous space of states: none
Bracket basis: none
Bracket rules: none
Hermitian operators: none
Unitary operators: none
Quantum operators: none
Algebra rules: none
Representation for the Dirac matrices: none
Default setup
User setup
Advanced setup
Apply to Session
Apply Globally
Cancel
Help
Now set L, p, r as quantum operators and the related Commutator rules for the algebra in tensor notation
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$$[automaticsimplification = true, metric = \{(1, 1) = 1, (2, 2) = 1, (3, 3) = 1, (4, 4) = 1\}, spaceindices = lowercaselatin] \quad (8)$$

Define $L$, $r$ and $p$ as tensors of the 3-D Euclidean space embedded in

> $Define(L, r, p)$

*Defined objects with tensor properties*

$$\{L, p, r, \gamma_{\mu}, \sigma_{\mu}, \partial_{\mu}, g_{\mu, \nu}, \gamma_{a, b}, \delta_{\mu, \nu}, \epsilon_{\alpha, \beta, \mu, \nu}\} \quad (9)$$

Now set $L$, $p$, $r$ as quantum operators and the related **Commutator** rules for the algebra in tensor notation

> $Setup(quantumoperators = \{L, p, r\},$
> $\{\%Commutator(p[j], p[k]) = 0,$
> $\%Commutator(r[j], p[k]) = i\ KroneckerDelta[j, k],$
> $\%Commutator(r[j], r[k]) = 0\})$

$$\left[algebrarules = \{[p_j, p_k]_- = 0, [r_j, p_k]_- = \mathrm{i}\,\delta_{j,k}, [r_j, r_k]_- = 0\}, quantumoperators = \{L, p, r\}\right] \quad (10)$$

The definition of $L_j$

> $L[j] = \mathrm{LeviCivita}[j, k, m]\ r[k]\ p[m]$

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Define $L, r$ and $p$ as tensors of the 3-D Euclidean space embedded in

> $Define(L, r, p)$

*Defined objects with tensor properties*

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> $\%Commutator(r[j], r[k]) = 0\})$

$$\left[algebrarules = \left\{ [p_j, p_k]_- = 0, [r_j, p_k]_- = i\,\delta_{j,k}, [r_j, r_k]_- = 0 \right\}, quantumoperators = \{L, p, r\}\right] \quad (10)$$

The definition of $L_j$

> $L[j] = \text{LeviCivita}[j, k, m]\ r[k]\,p[m]$

The rule to be verified:

> $\%Commutator(L[j], L[k]) = \mathrm{i}\ \text{LeviCivita}[j, k, m]\ L[m]$

Substitute now the operator $L_i$ by its tensor form in terms $r_k$ and $p_m$ in the commutator above

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{%Commutator(p[j], p[k]) = 0,
%Commutator(r[j], p[k]) = i KroneckerDelta[j, k],
%Commutator(r[j], r[k]) = 0})

$$\left[algebrarules = \left\{ \left[p_j, p_k\right]_- = 0, \left[r_j, p_k\right]_- = \mathrm{i}\, \delta_{j,k}, \left[r_j, r_k\right]_- = 0 \right\}, quantumoperators = \{L, p, r\}\right] \qquad (10)$$

The definition of $L_j$

> L[j] = LeviCivita[j, k, m] r[k] p[m]

$$L_j = \epsilon_{j,k,m} r_k p_m \qquad (11)$$

The rule to be verified:

> %Commutator(L[j], L[k]) = i LeviCivita[j, k, m] L[m]

$$\left[L_j, L_k\right]_- = \mathrm{i}\, \epsilon_{j,k,m} L_m \qquad (12)$$

Substitute now the operator $L_i$ by its tensor form in terms $r_k$ and $p_m$ in the commutator above

> Library:-SubstituteTensor((11), (12))

$$\left[\epsilon_{j,a,m} r_a p_m, \epsilon_{k,b,c} r_b p_c\right]_- = \mathrm{i}\, \epsilon_{m,a,b} r_a p_b \epsilon_{j,k,m} \qquad (13)$$

Simplify, all in one go, we expect an identity

> Simplify((13))

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The rule to be verified:

> *%Commutator*( $L[j], L[k]$ ) = i LeviCivita[ $j, k, m$ ] $L[m]$

$$[L_j, L_k]_- = \mathrm{i}\, \epsilon_{j,k,m} L_m \tag{12}$$

Substitute now the operator $L_i$ by its tensor form in terms $r_k$ and $p_m$ in the commutator above

> *Library:-SubstituteTensor*( **(11)**, **(12)** )

$$[\epsilon_{j,a,m} r_a p_m, \epsilon_{k,b,c} r_b p_c]_- = \mathrm{i}\, \epsilon_{m,a,b} r_a p_b \epsilon_{j,k,m} \tag{13}$$

Simplify, all in one go, we expect an identity

> *Simplify*( **(13)** )

$$\mathrm{i}\,(r_j p_k - r_k p_j) = \mathrm{i}\,(r_j p_k - r_k p_j) \tag{14}$$

The same one step at a time, first expand the commutator on the left-hand side

> *expand*( **(13)** )

$$-\epsilon_{a,j,m} \epsilon_{b,c,k} (r_a p_m r_b p_c - r_b p_c r_a p_m) = \mathrm{i}\, \epsilon_{a,b,m} r_a p_b \epsilon_{j,k,m} \tag{15}$$

> *Simplify*( **(15)** )

$$\mathrm{i}\,(r_j p_k - r_k p_j) = \mathrm{i}\,(r_j p_k - r_k p_j) \tag{16}$$

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> $Define(L, r, p)$

*Defined objects with tensor properties*

$$\{L, p, r, \gamma_{\mu}, \sigma_{\mu}, \partial_{\mu}, g_{\mu,\nu}, \gamma_{a,b}, \delta_{\mu,\nu}, \epsilon_{\alpha,\beta,\mu,\nu}\} \quad (9)$$

Now set $L$, $p$, $r$ as quantum operators and the related **Commutator** rules for the algebra in tensor notation

> $Setup(quantumoperators = \{L, p, r\},$
> $\{\%Commutator(p[j], p[k]) = 0,$
> $\%Commutator(r[j], p[k]) = i\, KroneckerDelta[j, k],$
> $\%Commutator(r[j], r[k]) = 0\})$

$$\left[algebrarules = \left\{ [p_j, p_k]_{-} = 0, [r_j, p_k]_{-} = \mathrm{i}\, \delta_{j,k}, [r_j, r_k]_{-} = 0 \right\}, quantumoperators = \{L, p, r\}\right] \quad (10)$$

The definition of $L_j$

> $L[j] = \mathrm{LeviCivita}[j, k, m]\ r[k]\, p[m]$

$$L_j = \epsilon_{j,k,m}\, r_k\, p_m \quad (11)$$

The rule to be verified:

> $\%Commutator(L[j], L[k]) = \mathrm{i}\ \mathrm{LeviCivita}[j, k, m]\ L[m]$

> $L[j] = \text{LeviCivita}[j, k, m]\ r[k]\, p[m]$

$$L_j = \epsilon_{j, k, m}\, r_k\, p_m \tag{11}$$

The rule to be verified:

> $\%Commutator(L[j], L[k]) = \mathrm{i}\ \text{LeviCivita}[j, k, m]\ L[m]$

$$[L_j, L_k]_- = \mathrm{i}\, \epsilon_{j, k, m}\, L_m \tag{12}$$

Substitute now the operator $L_i$ by its tensor form in terms $r_k$ and $p_m$ in the commutator above

> $Library\text{:-}SubstituteTensor(\mathbf{(11)}, \mathbf{(12)})$

$$[\epsilon_{j, a, m}\, r_a\, p_m, \epsilon_{k, b, c}\, r_b\, p_c]_- = \mathrm{i}\, \epsilon_{m, a, b}\, r_a\, p_b\, \epsilon_{j, k, m} \tag{13}$$

Simplify, all in one go, we expect an identity

> $Simplify(\mathbf{(13)})$

$$\mathrm{i}\,(r_j\, p_k - r_k\, p_j) = \mathrm{i}\,(r_j\, p_k - r_k\, p_j) \tag{14}$$

The same one step at a time, first expand the commutator on the left-hand side

> $expand(\mathbf{(13)})$

$$-\epsilon_{a, j, m}\, \epsilon_{b, c, k}\,(r_a\, p_m\, r_b\, p_c - r_b\, p_c\, r_a\, p_m) = \mathrm{i}\, \epsilon_{a, b, m}\, r_a\, p_b\, \epsilon_{j, k, m} \tag{15}$$

> $Simplify(\mathbf{(15)})$

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$$\left[\epsilon_{j, a, m}\, r_a\, p_m, \epsilon_{k, b, c}\, r_b\, p_c\right]_- = \mathrm{i}\, \epsilon_{m, a, b}\, r_a\, p_b\, \epsilon_{j, k, m} \quad (13)$$

Simplify, all in one go, we expect an identity

> *Simplify*((**13**))

$$\mathrm{i}\left(r_j p_k - r_k p_j\right) = \mathrm{i}\left(r_j p_k - r_k p_j\right) \quad \textbf{(14)}$$

The same one step at a time, first expand the commutator on the left-hand side

> *expand*((**13**))

$$-\epsilon_{a, j, m}\, \epsilon_{b, c, k}\left(r_a p_m r_b p_c - r_b p_c r_a p_m\right) = \mathrm{i}\, \epsilon_{a, b, m}\, r_a p_b\, \epsilon_{j, k, m} \quad \textbf{(15)}$$

> *Simplify*((**15**))

$$\mathrm{i}\left(r_j p_k - r_k p_j\right) = \mathrm{i}\left(r_j p_k - r_k p_j\right) \quad \textbf{(16)}$$

>

# Unitary Operators in Quantum Mechanics

(with Pascal Szriftgiser, from Laboratoire PhLAM, Université Lille 1, France)

## Eigenvalues of an unitary operator and exponential of Hermitian operators

## Properties of unitary operators

## Schrödinger equation and unitary transform

## Translation operators using Dirac notation

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> expand((15))

$$-\epsilon_{a,j,m}\,\epsilon_{b,c,k}\left(r_a p_m r_b p_c - r_b p_c r_a p_m\right) = \mathrm{i}\,\epsilon_{a,b,m}\, r_a p_b\, \epsilon_{j,k,m} \quad (15)$$

> *Simplify*((**15**))

$$\mathrm{i}\left(r_j p_k - r_k p_j\right) = \mathrm{i}\left(r_j p_k - r_k p_j\right) \quad (16)$$

>

## Unitary Operators in Quantum Mechanics

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- Eigenvalues of an unitary operator and exponential of Hermitian operators
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## Schrödinger vs Heisenberg picture

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# Classical Field Theory

# General Relativity

$$-\epsilon_{a,j,m}\,\epsilon_{b,c,k}\left(r_a\,p_m\,r_b\,p_c - r_b\,p_c\,r_a\,p_m\right) = \mathrm{i}\,\epsilon_{a,b,m}\,r_a\,p_b\,\epsilon_{j,k,m} \qquad (15)$$

> *Simplify*((**15**))

$$\mathrm{i}\left(r_j\,p_k - r_k\,p_j\right) = \mathrm{i}\left(r_j\,p_k - r_k\,p_j\right) \qquad (16)$$

>

# Unitary Operators in Quantum Mechanics

(with Pascal Szriftgiser, from Laboratoire PhLAM, Université Lille 1, France)

## Eigenvalues of an unitary operator and exponential of Hermitian operators

- Show that the eigenvalues of an unitary operator are all on the unit circle, their modulus is 1.
- Show that an operator $e^{i\lambda H}$ is unitary provided that $H$ is Hermitian ($H = H^{\dagger}$) and $\lambda$ is any real parameter.

***Solution***

## Properties of unitary operators

## Schrödinger equation and unitary transform

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> $restart; with(Physics) : interface(imaginaryunit = i) :$

> $Setup(unitaryoperators = \{U\})$

If $| U_{\varepsilon} \rangle$ is a normalized eigenvector of $U$ with eigenvalue ε

> $U \cdot Ket(U, \varepsilon) = U \cdot Ket(U, \varepsilon)$

> $Dagger(??)$

So, to show that the eigenvalues have modulus equal to 1, multiplying sides by sides

> ?? . ??

To show that, when $H$ is Hermitian, then $V = e^{i \lambda H}$ is unitary,

> $Setup(quantumoperators = \{V\}, hermitianoperators = \{H\}, realobjects = \{\lambda\})$

> $V = \exp(i \cdot \lambda \cdot H)$

> $Dagger(??)$

Again multiply sides by sides

> ?? . ??

> ?? . ??

Therefore, $V$ is unitary

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> $restart;\ with(Physics) : interface(imaginaryunit = i) :$

> $Setup(unitaryoperators = \{U\})$

$$[unitaryoperators = \{U\}] \tag{17}$$

If $|U_\varepsilon\rangle$ is a normalized eigenvector of $U$ with eigenvalue $\varepsilon$

> $U \cdot Ket(U, \varepsilon) = U \cdot Ket(U, \varepsilon)$

$$U |U_\varepsilon\rangle = \varepsilon |U_\varepsilon\rangle \tag{18}$$

> $Dagger(\mathbf{(18)})$

$$\langle U_\varepsilon | U^\dagger = \bar{\varepsilon} \langle U_\varepsilon | \tag{19}$$

So, to show that the eigenvalues have modulus equal to 1, multiplying sides by sides

> $\mathbf{(19)} \,.\, \mathbf{(18)}$

$$1 = |\varepsilon|^2 \tag{20}$$

To show that, when $H$ is Hermitian, then $V = e^{i \lambda H}$ is unitary,

> $Setup(quantumoperators = \{V\}, hermitianoperators = \{H\}, realobjects = \{\lambda\})$

> $V = \exp(i \cdot \lambda \cdot H)$

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$$1 = |\varepsilon|^2 \quad (20)$$

To show that, when $H$ is Hermitian, then $V = e^{i\lambda H}$ is unitary,

> $Setup(quantumoperators = \{V\}, hermitianoperators = \{H\}, realobjects = \{\lambda\})$

$$[hermitianoperators = \{H\}, quantumoperators = \{H, U, V\}, realobjects = \{\lambda\}] \quad (21)$$

> $V = \exp(i \cdot \lambda \cdot H)$

$$V = e^{i\lambda H} \quad (22)$$

> $Dagger(\mathbf{(22)})$

$$V^{\dagger} = e^{-i\lambda H} \quad (23)$$

Again multiply sides by sides

> $\mathbf{(22)} \cdot \mathbf{(23)}$

$$V V^{\dagger} = 1 \quad (24)$$

> $\mathbf{(23)} \cdot \mathbf{(22)}$

$$V^{\dagger} V = 1 \quad (25)$$

Therefore, $V$ is unitary

>

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> (22) . (23)

$$V V^{\dagger} = 1 \quad (24)$$

> (23) . (22)

$$V^{\dagger} V = 1 \quad (25)$$

Therefore, $V$ is unitary

>

▶ Properties of unitary operators

▶ Schrödinger equation and unitary transform

▶ Translation operators using Dirac notation

▶ Schrödinger vs Heisenberg picture

▶ Quantization of the energy of a particle in a magnetic field

▶ Quantization of the Lorentz Force

# ▶ Classical Field Theory

# ▶ General Relativity

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Consider two set of kets $|a_n\rangle$ and $|b_n\rangle$; each of them constituting a complete orthonormal basis *of the same space.*

- **Verify that* $U \equiv \sum_{k=0}^{\infty} |b_k\rangle\langle a_k|$; *maps one basis to the other, i.e.:* $|b_n\rangle \equiv U|a_n\rangle$
- **Show that* $U \equiv \sum_{k=0}^{\infty} |b_k\rangle\langle a_k|$ *is unitary*
- **Show that the matrix elements of U in the* $|a_n\rangle$ *and* $|b_n\rangle$ *basis are equal*
- *Show that* $A$ **and** $\mathcal{A} \equiv U\,A\,U^{\dagger}$ *have the same spectrum (eigenvalues)*

- Schrödinger equation and unitary transform
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# Classical Field Theory

# General Relativity

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## Properties of unitary operators

Consider two set of kets $|\, a_n \rangle$ and $|\, b_n \rangle$, each of them constituting a complete orthonormal basis *of the same space.*

- **Verify that* $U = \sum_{k=0}^{\infty} |\, b_k \rangle \langle\, a_k \,|$*, maps one basis to the other, i.e.:* $|\, b_n \rangle = U \,|\, a_n \rangle$
- **Show that* $U = \sum_{k=0}^{\infty} |\, b_k \rangle \langle\, a_k \,|$ *is unitary*
- **Show that the matrix elements of U in the* $|\, a_n \rangle$ *and* $|\, b_n \rangle$ *basis are equal*
- *Show that* $A$ **and** $\mathcal{A} = U\, A\, U^{\dagger}$ *have the same spectrum (eigenvalues)*

## Schrödinger equation and unitary transform

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# Classical Field Theory

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> restart; with(Physics) :

Tell the system that $|a_n\rangle$ and $|b_n\rangle$, are complete orthonormal basis

> $Setup(quantumoperators = \{U\},$
$bracketrules = \{\%Bracket(Bra(a, m), Ket(a, n)) = KroneckerDelta[m, n], \%Bracket(Bra(b, m), Ket(b, n))$
$= KroneckerDelta[m, n]\})$

$$\left[bracketrules = \left\{\langle a_m | a_n \rangle = \delta_{m,n}, \langle b_m | b_n \rangle = \delta_{m,n}\right\}, quantumoperators = \{U\}\right] \tag{26}$$

> $U = \sum_{k=0}^{\infty} Ket(b, k)\ Bra(a, k)$

$$U = \sum_{k=0}^{\infty} |b_k\rangle \langle a_k| \tag{27}$$

Apply this operatorial equation to $|a_m\rangle$

> $'\% .\ Ket(a, m)'$

$$\left(U = \sum_{k=0}^{\infty} |b_k\rangle \langle a_k|\right) \cdot |a_m\rangle \tag{28}$$

> %

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> Dagger((27))

$$U^{\dagger} = \sum_{k=0}^{\infty} | a_k \rangle \langle b_k | \quad (31)$$

Again multiply sides by sides

> '(31) . (27)'

$$\left(U^{\dagger} = \sum_{k=0}^{\infty} | a_k \rangle \langle b_k |\right) \cdot \left(U = \sum_{k=0}^{\infty} | b_k \rangle \langle a_k |\right) \quad (32)$$

> %

$$U^{\dagger} U = \sum_{k1=0}^{\infty} | a_{k1} \rangle \langle a_{k1} | \quad (33)$$

> (27) . (31)

$$U U^{\dagger} = \sum_{k1=0}^{\infty} | b_{k1} \rangle \langle b_{k1} | \quad (34)$$

and since $| a_n \rangle$ and $| b_n \rangle$ form two complete basis *of the same space*, the right-hand sides are equal to the identity operator $\mathbb{I}$, and so $U$ is unitary.

>

\> %

$$\langle a_n | U | a_m \rangle = \langle a_n | b_m \rangle \qquad (37)$$

Likewise

\> $Bra(b, n) . \mathbf{(27)} . Ket(b, m)$

$$\langle b_n | U | b_m \rangle = \langle a_n | b_m \rangle \qquad (38)$$

\>

▶ *Show that* $A$ **and** $\mathcal{A} = U\, A\, U^\dagger$ *have the same spectrum (eigenvalues)*

▶ Schrödinger equation and unitary transform

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$$i\,\hbar\,\frac{d}{dt}\left|\psi_t\right\rangle = H\left|\psi_t\right\rangle$$

where $H$, the Hamiltonian, as well as the quantum operators $O_S$ representing observable quantities, are all time-independent.

Within the Heisenberg picture, a Ket $\left|\psi\right\rangle$ representing the state of the system *does not evolve with time*, but the operators $O_H(t)$ representing observable quantities, and *through them* the Hamiltonian $H$, do.

**Problem:** Departing from Schrödinger's equation,

a) Show that the expected value of a physical observable in Schrödinger's and Heisenberg's representations is the same, i. e. that

$$\left\langle \psi_t \right| O_S \left| \psi_t \right\rangle = \left\langle \psi \right| O_H(t) \left| \psi \right\rangle$$

b) Show that the evolution equation of an observable $O_H$ in Heisenberg's picture, equivalent to Schrödinger's equation, is given by:

$$\dot{O}_H(t) = \frac{-i\left[O_H(t), H\right]_-}{\hbar}$$

where in the right-hand-side we see the commutator of $O_H$ with the Hamiltonian of the system.

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where $\vec{v}$ is the quantized velocity of the particle, and all of $H, \vec{p}, \vec{v}, \vec{B}, \vec{A}$ and $\vec{F}$ are Hermitian quantum operators representing observable quantities.

In the *classic (non-quantum) case*, the Lorentz force $\vec{F}$ for such a particle in the absence of electrical field is given by

$$\vec{F} = q\,\vec{v} \times \vec{B},$$

**Problem:** Departing from the Hamiltonian, show that in the *quantum case* the Lorentz force is given by

$$\vec{F} = \frac{q\left(\vec{v} \times \vec{B} - \vec{B} \times \vec{v}\right)}{2}$$

[1] Photons et atomes, Introduction à l'électrodynamique quantique, p. 179, Claude Cohen-Tannoudji, Jacques Dupont-Roc et Gilbert Grynberg - EDP Sciences janvier 1987.

>

▶ ***Solution***

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$$\vec{F} = q\,\vec{v} \times \vec{B}\,,$$

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▶ ***Solution***

▶ ***Solution***

# ▶ Classical Field Theory

▶ Classical Field Theory

# ▶ General Relativity

▶ General Relativity

# ▶ Tackling some Physical Review paper's computations

▶ Tackling some Physical Review paper's computations

# ▶ The Physics Project and what's next

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$$\vec{F} = q\,\vec{v} \times \vec{B}\,,$$

**Problem:** Departing from the Hamiltonian, show that in the *quantum case* the Lorentz force is given by

$$\vec{F} = \frac{q\,(\vec{v} \times \vec{B} - \vec{B} \times \vec{v})}{2}$$

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▶ ***Solution***

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$$\vec{F} = q\,\vec{v} \times \vec{B}\,,$$

**Problem:** Departing from the Hamiltonian, show that in the *quantum case* the Lorentz force is given by

$$\vec{F} = \frac{q\,(\vec{v} \times \vec{B} - \vec{B} \times \vec{v})}{2}$$

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>

▶ ***Solution***

# ▼ Classical Field Theory

▶ The field equations for the $\lambda\,\Phi^4$ model

▶ Maxwell equations departing from the 4-dimensional Action for Electrodynamics

▶ The field equations for a quantum system of identical particles

▶ General Relativity

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$$\vec{F} = \frac{q\,(\vec{v} \times \vec{B} - \vec{B} \times \vec{v})}{2}$$

[1] Photons et atomes, Introduction à l'électrodynamique quantique, p. 179, Claude Cohen-Tannoudji, Jacques Dupont-Roc et Gilbert Grynberg - EDP Sciences janvier 1987.

>

▶ ***Solution***

# ▼ Classical Field Theory

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Maxwell equations result from equation to zero the functional derivative o the Action with respect to the 4-D potential $A_{\mu}$

> *restart*; *with*(*Physics*) :

> *Coordinates*(*X*)

*Default differentiation variables for d_, D_ and dAlembertian are:* $\{X = (x1, x2, x3, x4)\}$

*Systems of spacetime Coordinates are:* $\{X = (x1, x2, x3, x4)\}$

$$\{X\} \tag{39}$$

The 4-D electromagnetic potential

> *Define*(*A*[mu](*X*))

> *CompactDisplay*(*A*(*X*))

The electromagnetic field tensor $F_{\mu, \nu}$

> *F*[mu, nu] := *d_*[mu](*A*[nu](*X*)) − *d_*[nu](*A*[mu](*X*));

Equate to 0 the functional derivative of the corresponding Action

> '*Fundiff*'(*Intc*(*F*[mu, nu]^2, *X*), *A*[rho]) = 0

> ??

> restart; with(Physics):

> $Coordinates(X)$

*Default differentiation variables for d_, D_ and dAlembertian are: {X = (x1, x2, x3, x4)}*

*Systems of spacetime Coordinates are: {X = (x1, x2, x3, x4)}*

$$\{X\} \quad (39)$$

The 4-D electromagnetic potential

> $Define(A[\mathrm{mu}](X))$

*Defined objects with tensor properties*

$$\left\{A_{\mu}, \gamma_{\mu}, \sigma_{\mu}, X_{\mu}, \partial_{\mu}, g_{\mu,\nu}, \delta_{\mu,\nu}, \epsilon_{\alpha,\beta,\mu,\nu}\right\} \quad (40)$$

> $CompactDisplay(A(X))$

$$A(X) \text{ will now be displayed as } A \quad (41)$$

The electromagnetic field tensor $F_{\mu,\nu}$

> $F[\mathrm{mu}, \mathrm{nu}] := d\_[\mathrm{mu}](A[\mathrm{nu}](X)) - d\_[\mathrm{nu}](A[\mathrm{mu}](X));$

$$F_{\mu,\nu} := \partial_{\mu}(A_{\nu}) - \partial_{\nu}(A_{\mu}) \quad (42)$$

Equate to 0 the functional derivative of the corresponding Action

> $'Fundiff'(Intc(F[\mathrm{mu}, \mathrm{nu}]^2, X), A[\mathrm{rho}]) = 0$

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> *CompactDisplay*( $A(X)$ )

$$A(X) \text{ will now be displayed as } A \quad \textbf{(41)}$$

The electromagnetic field tensor $F_{\mu, \nu}$

> $F[\text{mu}, \text{nu}] := d\_[\text{mu}](A[\text{nu}](X)) - d\_[\text{nu}](A[\text{mu}](X));$

$$F_{\mu, \nu} := \partial_\mu(A_\nu) - \partial_\nu(A_\mu) \quad \textbf{(42)}$$

Equate to 0 the functional derivative of the corresponding Action

> '*Fundiff*'( *Intc*( $F[\text{mu}, \text{nu}]$^2, $X$), $A[\text{rho}]$) = 0

> ??

Simplify the contracted spacetime indices

> *Simplify*( ?? )

The system of differential equations behind this formula in standard Maple notation:

> *OFF*; *convert*( *Library*:-*TensorComponents*( ?? ), *diff* )

>

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$$F_{\mu, \nu} := \partial_{\mu}(A_{\nu}) - \partial_{\nu}(A_{\mu}) \tag{42}$$

Equate to 0 the functional derivative of the corresponding Action

> 'Fundiff'(Intc(F[mu, nu]^2, X), A[rho]) = 0

$$\left(\frac{\delta}{\delta A_{\rho}}\right) \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\partial_{\mu}(A_{\nu}) - \partial_{\nu}(A_{\mu})\right)^2 \, dx1 \, dx2 \, dx3 \, dx4 = 0 \tag{43}$$

> (43)

$$\left(2\, \partial_{\mu}\left(\partial_{\nu}\left(A^{\nu}\right)\right) - 2\, \Box\left(A_{\mu}\right)\right) g^{\mu, \rho} + \left(-2\, \Box\left(A_{\nu}\right) + 2\, \partial_{\mu}\left(\partial_{\nu}\left(A^{\mu}\right)\right)\right) g^{\nu, \rho} = 0 \tag{44}$$

Simplify the contracted spacetime indices

> Simplify((44))

$$-4\, \Box\left(A^{\rho}\right) + 4\, \partial^{\mu}\left(\partial^{\rho}\left(A_{\mu}\right)\right) = 0 \tag{45}$$

The system of differential equations behind this formula in standard Maple notation:

> OFF; convert(Library:-TensorComponents((45)), diff)

>

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$$-4\,\Box\left(A^{\rho}\right) + 4\,\partial^{\mu}\left(\partial^{\rho}\left(A_{\mu}\right)\right) = 0 \qquad \textbf{(45)}$$

The system of differential equations behind this formula in standard Maple notation:

> *OFF*; *convert*(*Library*:-*TensorComponents*(**(45)**), *diff*)

$$\begin{aligned}
\Big[ & 4 \frac{\partial^2}{\partial x1^2} A^{1}(X) + 4 \frac{\partial^2}{\partial x2^2} A^{1}(X) + 4 \frac{\partial^2}{\partial x3^2} A^{1}(X) - 4 \frac{\partial^2}{\partial x4^2} A^{1}(X) + 4 \frac{\partial^2}{\partial x1^2} A_{1}(X) + 4 \frac{\partial^2}{\partial x1 \partial x2} A_{2}(X) \\
& + 4 \frac{\partial^2}{\partial x1 \partial x3} A_{3}(X) - 4 \frac{\partial^2}{\partial x1 \partial x4} A_{4}(X) = 0,\ 4 \frac{\partial^2}{\partial x1^2} A^{2}(X) + 4 \frac{\partial^2}{\partial x2^2} A^{2}(X) + 4 \frac{\partial^2}{\partial x3^2} A^{2}(X) - 4 \frac{\partial^2}{\partial x4^2} \\
& A^{2}(X) + 4 \frac{\partial^2}{\partial x1 \partial x2} A_{1}(X) + 4 \frac{\partial^2}{\partial x2^2} A_{2}(X) + 4 \frac{\partial^2}{\partial x2 \partial x3} A_{3}(X) - 4 \frac{\partial^2}{\partial x2 \partial x4} A_{4}(X) = 0,\ 4 \frac{\partial^2}{\partial x1^2} A^{3}(X) \\
& + 4 \frac{\partial^2}{\partial x2^2} A^{3}(X) + 4 \frac{\partial^2}{\partial x3^2} A^{3}(X) - 4 \frac{\partial^2}{\partial x4^2} A^{3}(X) + 4 \frac{\partial^2}{\partial x1 \partial x3} A_{1}(X) + 4 \frac{\partial^2}{\partial x2 \partial x3} A_{2}(X) + 4 \frac{\partial^2}{\partial x3^2} \\
& A_{3}(X) - 4 \frac{\partial^2}{\partial x3 \partial x4} A_{4}(X) = 0,\ 4 \frac{\partial^2}{\partial x1^2} A^{4}(X) + 4 \frac{\partial^2}{\partial x2^2} A^{4}(X) + 4 \frac{\partial^2}{\partial x3^2} A^{4}(X) - 4 \frac{\partial^2}{\partial x4^2} A^{4}(X) \\
& - 4 \frac{\partial^2}{\partial x1 \partial x4} A_{1}(X) - 4 \frac{\partial^2}{\partial x2 \partial x4} A_{2}(X) - 4 \frac{\partial^2}{\partial x3 \partial x4} A_{3}(X) + 4 \frac{\partial^2}{\partial x4^2} A_{4}(X) = 0 \Big]
\end{aligned} \qquad \textbf{(46)}$$

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Equate to 0 the functional derivative of the corresponding Action

> *'Fundiff'*(*Intc*(*F*[mu, nu]^2, *X*), *A*[rho]) = 0

$$\left(\frac{\delta}{\delta A_{\rho}}\right)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\partial_{\mu}(A_{\nu})-\partial_{\nu}(A_{\mu})\right)^{2}\,\mathrm{d}x1\,\mathrm{d}x2\,\mathrm{d}x3\,\mathrm{d}x4=0 \quad \textbf{(43)}$$

> **(43)**

$$\left(2\,\partial_{\mu}\left(\partial_{\nu}\left(A^{\nu}\right)\right)-2\,\Box\left(A_{\mu}\right)\right)g^{\mu,\rho}+\left(-2\,\Box\left(A_{\nu}\right)+2\,\partial_{\mu}\left(\partial_{\nu}\left(A^{\mu}\right)\right)\right)g^{\nu,\rho}=0 \quad \textbf{(44)}$$

Simplify the contracted spacetime indices

> *Simplify*(**(44)**)

$$-4\,\Box\left(A^{\rho}\right)+4\,\partial^{\mu}\left(\partial^{\rho}\left(A_{\mu}\right)\right)=0 \quad \textbf{(45)}$$

The system of differential equations behind this formula in standard Maple notation:

> *OFF*; *convert*(*Library*:-*TensorComponents*(**(45)**), *diff*)

$$\left[4\,\frac{\partial^2}{\partial x1^2}A^{1}(X)+4\,\frac{\partial^2}{\partial x2^2}A^{1}(X)+4\,\frac{\partial^2}{\partial x3^2}A^{1}(X)-4\,\frac{\partial^2}{\partial x4^2}A^{1}(X)+4\,\frac{\partial^2}{\partial x1^2}A_{1}(X)+4\,\frac{\partial^2}{\partial x1\partial x2}A_{2}(X)\right. \quad \textbf{(46)}$$

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$$-4\frac{\partial^2}{\partial x1 \partial x4}A_1(X)-4\frac{\partial^2}{\partial x2 \partial x4}A_2(X)-4\frac{\partial^2}{\partial x3 \partial x4}A_3(X)+4\frac{\partial^2}{\partial x4^2}A_4(X)=0\Big]$$

>

# The field equations for a quantum system of identical particles

**Problem:** derive the field equation describing the ground state of a quantum system of identical particles (bosons), that is, the Gross-Pitaevskii equation (GPE). This equation is particularly useful to describe Bose-Einstein condensates (BEC).

## Solution

Two steps:

- Construct the Lagrangian for the system, and with it write the action functional
- Minimize the action by equating to zero its functional derivative with respect to the boson field.

```
> restart; with(Physics) : with(Physics[Vectors]) :
> interface(imaginaryunit = i) :
> macro(Psi = psi(x, y, z, t)) :
> PDEtools:-declare((ψ, V)(x, y, z, t))
```

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$$E := \frac{\hbar^2 \|\nabla\psi\|^2}{2\,m} + V\,|\psi|^2 + \frac{G\,|\psi|^4}{2} \quad (48)$$

$\psi(x, y, z, t)$ is a complex field, $V(x, y, z, t)$ an external potential, the term $\frac{G\,|\psi|^4}{2}$ is the atom-atom interaction.

> $Setup(realobjects = \{t, m, \hbar, G, V(x, y, z, t)\})$ :

The Lagrangian density $L$ in terms of the Energy $E$

> $L := \left(\frac{i\,\hbar}{2}\right)(conjugate(\mathrm{Psi})\,diff(\mathrm{Psi}, t) - \mathrm{Psi}\,diff(conjugate(\mathrm{Psi}), t)) - E$

$$L := \frac{\mathrm{i}\,\hbar\,(\overline{\psi}\,\psi_t - \psi\,\overline{\psi}_t)}{2} - \frac{\hbar^2 \|\nabla\psi\|^2}{2\,m} - V\,|\psi|^2 - \frac{G\,|\psi|^4}{2} \quad (49)$$

Construct the action and equate to zero the functional derivative

> $'Fundiff'(Intc(L, x, y, z, t), \mathrm{psi}) = 0$

$$\left(\frac{\delta}{\delta\,\psi}\right)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{\mathrm{i}\,\hbar\,(\overline{\psi}\,\psi_t - \psi\,\overline{\psi}_t)}{2} - \frac{\hbar^2 \|\nabla\psi\|^2}{2\,m} - V\,|\psi|^2 - \frac{G\,|\psi|^4}{2}\right) \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}t = 0 \quad (50)$$

> **(50)**

Construct the action and equate to zero the functional derivative

> 'Fundiff'(Intc(L, x, y, z, t), psi) = 0

$$\left(\frac{\delta}{\delta\,\psi}\right)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{i\,\hbar\,\left(\overline{\psi}\,\psi_t-\psi\,\overline{\psi}_t\right)}{2}-\frac{\hbar^2\,\|\nabla\psi\|^2}{2\,m}-V\,|\psi|^2-\frac{G\,|\psi|^4}{2}\right)\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}t=0 \quad \textbf{(50)}$$

> (50)

$$\frac{\hbar^2\,\overline{\psi}_{x,x}+\overline{\psi}_{y,y}\,\hbar^2+\hbar^2\,\overline{\psi}_{z,z}-2\left(G\,\overline{\psi}^2\,\psi+i\,\overline{\psi}_t\,\hbar+\overline{\psi}\,V\right)m}{2\,m}=0 \quad \textbf{(51)}$$

Make the Laplacian explicit

> (Laplacian = %Laplacian)(Psi)

$$\psi_{x,x}+\psi_{y,y}+\psi_{z,z}=\nabla^2\psi \quad \textbf{(52)}$$

> simplify(conjugate((51)), {(52)})

The standard form of the Gross–Pitaevskii equation:

> i ℏ isolate(??, diff(Psi, t))

> collect(convert(expand(??), abs), psi)

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$$\frac{\ldots}{2\,m} = 0 \qquad (51)$$

Make the Laplacian explicit

> $(Laplacian = \%Laplacian)(\mathrm{Psi})$

$$\psi_{x,x} + \psi_{y,y} + \psi_{z,z} = \nabla^2\psi \qquad (52)$$

> $simplify(conjugate((\mathbf{51})), \{(\mathbf{52})\})$

$$\frac{2\,\mathrm{i}\,\hbar\,\psi_t\,m + \hbar^2\,\nabla^2\psi - 2\,m\,\psi\,(G\,\overline{\psi}\,\psi + V)}{2\,m} = 0 \qquad (53)$$

The standard form of the Gross–Pitaevskii equation:

> $i\,\hbar\,isolate((\mathbf{53}), diff(\mathrm{Psi}, t))$

$$\mathrm{i}\,\psi_t\,\hbar = \frac{-\hbar^2\,\nabla^2\psi + 2\,m\,\psi\,(G\,\overline{\psi}\,\psi + V)}{2\,m} \qquad (54)$$

> $collect(convert(expand((\mathbf{54})), \mathrm{abs}), \mathrm{psi})$

$$\mathrm{i}\,\psi_t\,\hbar = \left(G\,|\psi|^2 + V\right)\psi - \frac{\hbar^2\,\nabla^2\psi}{2\,m} \qquad (55)$$

>

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> collect(convert(expand((54)), abs), psi)

$$i\,\psi_t\,\hbar = \left(G\,|\psi|^2 + V\right)\psi - \frac{\hbar^2\,\nabla^2\psi}{2\,m} \quad (55)$$

>

# General Relativity

## Database of solutions to Einstein's Equations $G_{\mu,\nu} + g_{\mu,\nu}\,\Lambda = 8\,\pi\,T_{\mu,\nu}$

Main reference: - Stephani, H., Kramer, D., MacCallum, M., Hoenselaers, C. Herlt, E. **Exact Solutions of Einstein's Field Equations**, Cambridge Monographs on Mathematical Physics, second edition. Cambridge University Press, 2003.

*The authors reviewed more than **4,000 papers containing solutions to Einstein's equations** in the literature and organized the material into chapters according to the physical properties of these solutions.*

These solutions are digitized within Maple since 2016, so that ***it is now possible to actually compute with them***.

### *Examples*

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> g_[sc]

*Systems of spacetime Coordinates are:* $\{X = (r, \theta, \phi, t)\}$

*Default differentiation variables for d_, D_ and dAlembertian are:* $\{X = (r, \theta, \phi, t)\}$

*The Schwarzschild metric in coordinates* $[r, \theta, \phi, t]$

*Parameters:* $[m]$

$$g_{\mu, \nu} = \begin{bmatrix} \frac{r}{-r + 2\,m} & 0 & 0 & 0 \\ 0 & -r^2 & 0 & 0 \\ 0 & 0 & -r^2 \sin(\theta)^2 & 0 \\ 0 & 0 & 0 & \frac{r - 2\,m}{r} \end{bmatrix} \tag{56}$$

And that is all we do. Everything else gets automatically computed on background (the only information saved in the database is the metric)

The tensor components of the general relativity tensors related to this solution get derived automatically from their definition

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> g_[sc]

*Systems of spacetime Coordinates are:* $\{X=(r, \theta, \phi, t)\}$

*Default differentiation variables for d_, D_ and dAlembertian are:* $\{X=(r, \theta, \phi, t)\}$

*The Schwarzschild metric in coordinates* $[r, \theta, \phi, t]$

*Parameters:* $[m]$

$$g_{\mu, \nu} = \begin{bmatrix} \frac{r}{-r+2m} & 0 & 0 & 0 \\ 0 & -r^2 & 0 & 0 \\ 0 & 0 & -r^2 \sin(\theta)^2 & 0 \\ 0 & 0 & 0 & \frac{r-2m}{r} \end{bmatrix} \quad (56)$$

And that is all we do. Everything else gets automatically computed on background (the only information saved in the database is the metric)

The tensor components of the general relativity tensors related to this solution get derived automatically from their definition

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> *Christoffel*[ ~1, alpha, beta, *matrix* ]

$$\Gamma^{1}{}_{\alpha, \beta} = \begin{bmatrix} \frac{m}{r(-r+2m)} & 0 & 0 & 0 \\ 0 & -r+2m & 0 & 0 \\ 0 & 0 & (-r+2m)\sin(\theta)^2 & 0 \\ 0 & 0 & 0 & \frac{-2m^2+mr}{r^3} \end{bmatrix} \quad (58)$$

> *Riemann*[ *definition* ]

$$R_{\alpha, \beta, \mu, \nu} = g_{\alpha, \lambda}\left(\partial_{\mu}\left(\Gamma^{\lambda}{}_{\beta, \nu}\right) - \partial_{\nu}\left(\Gamma^{\lambda}{}_{\beta, \mu}\right) + \Gamma^{\lambda}{}_{\upsilon, \mu}\Gamma^{\upsilon}{}_{\beta, \nu} - \Gamma^{\lambda}{}_{\upsilon, \nu}\Gamma^{\upsilon}{}_{\beta, \mu}\right) \quad (59)$$

For example, the Riemann invariants using the standard formulas by Carminati and McLenaghan

> *Riemann*[ *invariants* ]

$$r_0 = 0, r_1 = 0, r_2 = 0, r_3 = 0, w_1 = \frac{6m^2}{r^6}, w_2 = \frac{6m^3}{r^9}, m_1 = 0, m_2 = 0, m_3 = 0, m_4 = 0, m_5 = 0 \quad (60)$$

The related Weyl scalars in the context of the Newman-Penrose formalism

> *Weyl*[ *scalarsdefinition* ]

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$$\Gamma_{\alpha,\beta} = \begin{bmatrix} \cdots \\ 0 & 0 & (-r+2m)\sin(\theta)^2 & 0 \\ 0 & 0 & 0 & \frac{-2m^2+mr}{r^3} \end{bmatrix} \quad (58)$$

> *Riemann[definition]*

$$R_{\alpha,\beta,\mu,\nu} = g_{\alpha,\lambda}\left(\partial_\mu\left(\Gamma^{\lambda}{}_{\beta,\nu}\right) - \partial_\nu\left(\Gamma^{\lambda}{}_{\beta,\mu}\right) + \Gamma^{\lambda}{}_{\upsilon,\mu}\Gamma^{\upsilon}{}_{\beta,\nu} - \Gamma^{\lambda}{}_{\upsilon,\nu}\Gamma^{\upsilon}{}_{\beta,\mu}\right) \quad (59)$$

For example, the Riemann invariants using the standard formulas by Carminati and McLenaghan

> *Riemann[invariants]*

$$r_0 = 0, r_1 = 0, r_2 = 0, r_3 = 0, w_1 = \frac{6m^2}{r^6}, w_2 = \frac{6m^3}{r^9}, m_1 = 0, m_2 = 0, m_3 = 0, m_4 = 0, m_5 = 0 \quad (60)$$

The related Weyl scalars in the context of the Newman-Penrose formalism

Help:Physics,Weyl

> *Weyl[scalarsdefinition]*

$$\Psi_0 = -C^{\mu,\nu,\alpha,\beta}\, l_\mu m_\nu l_\alpha m_\beta, \Psi_1 = -C^{\mu,\nu,\alpha,\beta}\, l_\mu n_\nu l_\alpha m_\beta, \Psi_2 = -C^{\mu,\nu,\alpha,\beta}\, l_\mu m_\nu \overline{m}_\alpha n_\beta, \Psi_3 = -C^{\mu,\nu,\alpha,\beta}\, l_\mu n_\nu \overline{m}_\alpha n_\beta, \Psi_4 = -C^{\mu,\nu,\alpha,\beta}\, n_\mu \overline{m}_\nu n_\alpha \overline{m}_\beta \quad (61)$$

> *Weyl[scalars]*

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$$g_{\alpha,\nu}\,\mathcal{D}_{\mu}\left(K^{\alpha}\right)+g_{\mu,\alpha}\,\mathcal{D}_{\nu}\left(K^{\alpha}\right) \quad (66)$$

> *TensorArray*((66))

$$\left[\left[0,0,0,0\right],\right. \quad (67)$$

$$\left[0,0,-r^2\sin(\theta)^2\left(-\frac{\cos(\phi)\left(1+\tan(\theta)^2\right)}{\tan(\theta)^2}+\frac{\cos(\theta)\cos(\phi)}{\sin(\theta)\tan(\theta)}\right)-r^2\left(\cos(\phi)-\frac{\sin(\theta)\cos(\theta)\cos(\phi)}{\tan(\theta)}\right),0\right],$$

$$\left[0,-r^2\sin(\theta)^2\left(-\frac{\cos(\phi)\left(1+\tan(\theta)^2\right)}{\tan(\theta)^2}+\frac{\cos(\theta)\cos(\phi)}{\sin(\theta)\tan(\theta)}\right)-r^2\left(\cos(\phi)-\frac{\sin(\theta)\cos(\theta)\cos(\phi)}{\tan(\theta)}\right),\right.$$

$$\left.-2\,r^2\sin(\theta)^2\left(-\frac{\sin(\phi)}{\tan(\theta)}+\frac{\cos(\theta)\sin(\phi)}{\sin(\theta)}\right),0\right],$$

$$\left[0,0,0,0\right]$$

> *simplify*((67))

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$$\textit{phi}(\tau) \text{ will now be displayed as } \phi$$

$$t(\tau) \text{ will now be displayed as } t \tag{70}$$

> Geodesics( )

$$\left[\phi_{\tau,\tau} = -\frac{2\,\phi_\tau\left(\cos(\theta)\,r\,\theta_\tau + \sin(\theta)\,r_\tau\right)}{r\sin(\theta)},\ \theta_{\tau,\tau} = \frac{\sin(\theta)\cos(\theta)\,\phi_\tau^{\,2}\,r - 2\,r_\tau\,\theta_\tau}{r},\ r_{\tau,\tau}\right. \tag{71}$$

$$= \frac{1}{(-r+2\,m)\,r^3}\left(4\,r^3\left(\cos(\theta)+1\right)\left(\cos(\theta)-1\right)\left(-\frac{r}{2}+m\right)^2\phi_\tau^{\,2} - 4\,r^3\left(-\frac{r}{2}+m\right)^2\theta_\tau^{\,2}\right.$$

$$\left. + 4\left(-\frac{r}{2}+m\right)^2 m\,t_\tau^{\,2} - m\,r_\tau^{\,2}\,r^2\right),\ t_{\tau,\tau} = -\frac{2\,m\,r_\tau\,t_\tau}{r\,(r-2\,m)},$$

This system of ODEs, as is, it is out of reach of the DE solvers of the system mainly due to the presence of non-rational objects like sin and cos having for arguments one of the unknowns of the system, $\theta(\tau)$. On the other hand, we know the geodesics for the Schwarzschild metric describe the motion of particles in the gravitational field of a central fixed large mass. So to investigate the solvability of these equations one can assume $\theta(\tau)$ is constant an due to the rotational symmetry choose a value for it that simplifies the equations, for example, $\theta(\tau) = \frac{\pi}{2}$.

> **(71)**

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$$\left[ \frac{2\, m\, r_{\tau}\, t_{\tau}}{r\,(r-2\,m)} \right.$$ ,

> $dsolve(\mathbf{(72)})[1..2]$ # *10 seconds ...*

$$[\{r=6\,m\}, \{\phi=\_C2\,\tau+\_C3\}, \{t=-6\sqrt{6}\,m\,\phi+\_C1, t=6\sqrt{6}\,m\,\phi+\_C1\}], \left[\{r=\_C4\}, \{\phi=\_C2\,\tau + \_C3\}, \left\{t=\int \frac{\sqrt{r\,m}\;r\,\phi_{\tau}}{m}\,\mathrm{d}\tau+\_C1, t=\int -\frac{\sqrt{r\,m}\;r\,\phi_{\tau}}{m}\,\mathrm{d}\tau+\_C1\right\}\right] \qquad \mathbf{(73)}$$

## Computational challenge (no meaning, just a test)

Load again Schwarzschild's solution, rewrite Einstein's equations ***in abstract form in terms of the metric*** $g_{\mu,\nu}$ ***and its derivatives***, and show that all the components of the *EnergyMomentum* tensor $T_{\mu,\nu}$ are equal to zero (Schwarzschild's solution in vacuum)

> $g\_[sc]$

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## Solution

### *Formulation of the problem*

Load the ThreePlusOne Physics package and the Lemaitre-Tolman-Bondi metric, that in the Maple database of solutions to Einstein's equations can be retrieved directly using a portion of the word Tolman as an index to the metric g_

> *restart*; *with*(*Physics*) : *with*(*ThreePlusOne*)

*Setting lowercaselatin_is letters to represent space indices*

*Defined as 4D, spacetime tensors that are purely spatial(see ?Physics,ThreePlusOne)*, $\gamma_{\mu, \nu}$, $\mathcal{D}_{\mu}$, $\Gamma_{\mu, \nu, \alpha}$, $\boldsymbol{R}_{\mu, \nu}$, $\boldsymbol{R}_{\mu, \nu, \alpha, \beta}$, $\beta_{\mu}$, $\boldsymbol{n}_{\mu}$, $\boldsymbol{t}_{\mu}$, $K_{\mu, \nu}$

*Changing the signature of spacetime from (- - - +) to (+ + + -) in order to match the signature customarily used in the ADM formalism*

[*ADMEquations*, *Christoffel3*, *D3_*, *ExtrinsicCurvature*, *Lapse*, *Ricci3*, *Riemann3*, *Shift*, *TimeVector*, *UnitNormalVector*, *gamma3_*] **(74)**

> $g_{-tol}$

> *CompactDisplay*( %% )

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$$\left[0 = 0, 0 = 0, -\rho_\Lambda R^2 \sin(\theta)^2 = -\frac{R \sin(\theta)^2 \left(R_{r,t,t} R + R_{t,t} R_r + R_t R_{r,t} - E_r\right)}{8 R_r \pi}, 0 = 0\right],$$

$$\left[0 = 0, 0 = 0, 0 = 0, \rho_M + \rho_\Lambda = -\frac{-2 R R_t R_{r,t} - R_r R_t^2 + 2 R E_r + 2 R_r E}{8 R_r R^2 \pi}\right]\Big]$$

Introduce $M(r)$, the gravitational mass of a sphere at radius $r$ (see wikipedia for definitions)

> $M(r) = -\frac{1}{2}\left(-\left(\frac{\partial}{\partial t} R(t, r)\right)^2 + 2 E(r)\right) R(t, r)$

$$M(r) = -\left(-\frac{R_t^2}{2} + E\right) R \quad \mathbf{(82)}$$

The relationship we are looking for is in $EQ4_{4,4}$, so simplify the expression obtained for $\rho_M + \rho_\Lambda$ introducing $M(r)$ and eliminating $E(r)$ (see simplify, siderelations)

> $simplify\left(EQ4_{4,4}, \{\mathbf{(82)}\}, \{E(r)\}\right)$

***b) Show that the 4D Einstein equations and their 3 + 1 split in terms of the extrinsic curvature are one and same system***

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The second equation, $eq_2$, is identically satisfied

> $eq_2$

$$\mathcal{D}_{\beta}\left(\mathbf{K}_{\mu}{}^{\beta}\right) - \gamma_{\mu}{}^{\tau}\Bigg( -\frac{1}{R_r R}\left(\partial_{\tau}(R)\, R_{r,t} + R\left(R_{r,r,t}\,\partial_{\tau}(r) + R_{r,t,t}\,\partial_{\tau}(t)\right) + 2\left(R_{r,r}\,\partial_{\tau}(r) + R_{r,t}\,\partial_{\tau}(t)\right) R_t + 2 R_r\left(R_{r,t}\,\partial_{\tau}(r) + R_{t,t}\,\partial_{\tau}(t)\right)\right) + \frac{\left(R\, R_{r,t} + 2 R_r R_t\right)\left(R_{r,r}\,\partial_{\tau}(r) + R_{r,t}\,\partial_{\tau}(t)\right)}{R_r^{\,2} R} + \frac{\left(R\, R_{r,t} + 2 R_r R_t\right)\partial_{\tau}(R)}{R_r R^2}\Bigg) = -8\pi\gamma_{\mu}{}^{\beta}\, n^{\tau}\, \mathrm{T}_{\beta,\tau} \tag{89}$$

> $TensorArray(eq_2, simplifier = simplify)$

$$\left[\; 0 = 0 \quad 0 = 0 \quad 0 = 0 \quad 0 = 0 \;\right] \tag{90}$$

The fourth equation, $eq_4$, is also identically satisfied (basically, this is the definition of the ExtrinsicCurvature)

> $eq_4$

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$$\beta, \tau \Big]$$

$$\Big[ t^{\tau} \mathcal{D}_{\tau}\left(\mathbf{K}_{\mu, \nu}\right) + \mathbf{K}_{\tau, \nu} \mathcal{D}_{\mu}\left(t^{\tau}\right) + \mathbf{K}_{\mu, \tau} \mathcal{D}_{\nu}\left(t^{\tau}\right) = -\frac{\left(R R_{r, t} + 2 R_{r} R_{t}\right) \mathbf{K}_{\mu, \nu}}{R_{r} R} - 2 \mathbf{K}_{\mu, \tau} \mathbf{K}^{\tau}{}_{\nu} + \boldsymbol{R}_{\mu, \nu}$$

$$- 8 \pi \left(\gamma_{\mu}{}^{\kappa} \gamma_{\nu}{}^{\lambda} \mathrm{T}_{\kappa, \lambda} - \frac{\gamma_{\mu, \nu}\left(\gamma_{\kappa}{}^{\lambda} \gamma^{\kappa, \sigma} \mathrm{T}_{\lambda, \sigma} - \mathrm{T}^{\alpha, \beta} \boldsymbol{n}_{\alpha} \boldsymbol{n}_{\beta}\right)}{2}\right) + \beta^{\tau} \mathcal{D}_{\tau}\left(\mathbf{K}_{\mu, \nu}\right) + \mathbf{K}_{\tau, \nu} \mathcal{D}_{\mu}\left(\beta^{\tau}\right)$$

$$+ \mathbf{K}_{\mu, \tau} \mathcal{D}_{\nu}\left(\beta^{\tau}\right) \Big]$$

$$\Big[ t^{\tau} \mathcal{D}_{\tau}\left(\gamma_{\mu, \nu}\right) + \gamma_{\tau, \nu} \mathcal{D}_{\mu}\left(t^{\tau}\right) + \gamma_{\mu, \tau} \mathcal{D}_{\nu}\left(t^{\tau}\right) = -2 \mathbf{K}_{\mu, \nu} + \beta^{\tau} \mathcal{D}_{\tau}\left(\gamma_{\mu, \nu}\right) + \gamma_{\tau, \nu} \mathcal{D}_{\mu}\left(\beta^{\tau}\right) + \gamma_{\mu, \tau} \mathcal{D}_{\nu}\left(\beta^{\tau}\right)$$

$$\Big]\Big]$$

The expression for $\rho_{M} + \rho_{\Lambda}$ in terms of $M(r)$ is obtained now from $eq_{1}$

> $eq_{1}$

> $eq_1$

$$\frac{\left(R\, R_{r,\,t} + 2\, R_r\, R_t\right)^2}{R_r^{\;2}\, R^2} - \mathbf{K}_{\alpha,\,\beta}\, \mathbf{K}^{\alpha,\,\beta} - \frac{4\left(R_r\, E + R\, E_r\right)}{R_r\, R^2} = 16\, \pi\, \boldsymbol{n}_{\alpha}\, \boldsymbol{n}_{\beta}\, \mathrm{T}^{\alpha,\,\beta} \tag{85}$$

> $SumOverRepeatedIndices(eq_1)$

$$\frac{2\left(2\, R\, R_t\, R_{r,\,t} + R_r\, R_t^{\;2} - 2\, R\, E_r - 2\, R_r\, E\right)}{R_r\, R^2} = 16\, \pi\left(\rho_M + \rho_\Lambda\right) \tag{86}$$

> $isolate\left(\mathbf{(86)},\, \rho_M(t, r) + \rho_\Lambda\right)$

$$\rho_M + \rho_\Lambda = \frac{2\, R\, R_t\, R_{r,\,t} + R_r\, R_t^{\;2} - 2\, R\, E_r - 2\, R_r\, E}{8\, R_r\, R^2\, \pi} \tag{87}$$

> $simplify(\mathbf{(87)},\, \{\mathbf{(82)}\},\, \{E(r)\})$

$$\rho_M + \rho_\Lambda = \frac{M_r}{4\, R^2\, R_r\, \pi} \tag{88}$$

The second equation, $eq_2$, is identically satisfied

> $eq_2$

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> $eq_1$

$$\frac{\left(R\, R_{r,\,t} + 2\, R_r\, R_t\right)^2}{R_r^{\,2}\, R^2} - \mathbf{K}_{\alpha,\,\beta}\, \mathbf{K}^{\alpha,\,\beta} - \frac{4\left(R_r\, E + R\, E_r\right)}{R_r\, R^2} = 16\, \pi\, \boldsymbol{n}_{\alpha}\, \boldsymbol{n}_{\beta}\, \mathrm{T}^{\alpha,\,\beta} \tag{85}$$

> $SumOverRepeatedIndices(eq_1)$

$$\frac{2\left(2\, R\, R_t\, R_{r,\,t} + R_r\, R_t^2 - 2\, R\, E_r - 2\, R_r\, E\right)}{R_r\, R^2} = 16\, \pi\left(\rho_M + \rho_\Lambda\right) \tag{86}$$

> $isolate(\mathbf{(86)}, \rho_M(t, r) + \rho_\Lambda)$

$$\rho_M + \rho_\Lambda = \frac{2\, R\, R_t\, R_{r,\,t} + R_r\, R_t^2 - 2\, R\, E_r - 2\, R_r\, E}{8\, R_r\, R^2\, \pi} \tag{87}$$

> $simplify(\mathbf{(87)}, \{\mathbf{(82)}\}, \{E(r)\})$

$$\rho_M + \rho_\Lambda = \frac{M_r}{4\, R^2\, R_r\, \pi} \tag{88}$$

The second equation, $eq_2$, is identically satisfied

> $eq_2$

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> $isolate\left((\mathbf{86}), \rho_M(t,r) + \rho_\Lambda\right)$

$$\rho_M + \rho_\Lambda = \frac{2\, R\, R_t\, R_{r,\,t} + R_r\, R_t^2 - 2\, R\, E_r - 2\, R_r\, E}{8\, R_r\, R^2\, \pi} \qquad (87)$$

> $simplify\left((\mathbf{87}), \{(\mathbf{82})\}, \{E(r)\}\right)$

$$\rho_M + \rho_\Lambda = \frac{M_r}{4\, R^2\, R_r\, \pi} \qquad (88)$$

The second equation, $eq_2$, is identically satisfied

> $eq_2$

> $TensorArray\left(eq_2, simplifier = simplify\right)$

The fourth equation, $eq_4$, is also identically satisfied (basically, this is the definition of the ExtrinsicCurvature)

> $eq_4$

> $TensorArray\left(eq_2, simplifier = simplify\right)$

So it is in $eq_1$ where the evolution of the gravitational field is encoded, in terms of the functions $\{\rho_M, E(r), R(t,r)\}$

$$8\, R_r\, R^2\, \pi$$

> $simplify(\mathbf{(87)}, \{\mathbf{(82)}\}, \{E(r)\})$

$$\rho_M + \rho_\Lambda = \frac{M_r}{4\, R^2\, R_r\, \pi} \quad \mathbf{(88)}$$

The second equation, $eq_2$, is identically satisfied

> $eq_2$

$$\mathcal{D}_\beta\left(\mathbf{K}_\mu{}^\beta\right) - \gamma_\mu{}^\tau \Bigg( -\frac{1}{R_r\, R}\Big(\partial_\tau(R)\, R_{r,t} + R\left(R_{r,r,t}\,\partial_\tau(r) + R_{r,t,t}\,\partial_\tau(t)\right) + 2\left(R_{r,r}\,\partial_\tau(r) + R_{r,t}\,\partial_\tau(t)\right) R_t + 2\, R_r\left(R_{r,t}\,\partial_\tau(r) + R_{t,t}\,\partial_\tau(t)\right)\Big) + \frac{\left(R\, R_{r,t} + 2\, R_r\, R_t\right)\left(R_{r,r}\,\partial_\tau(r) + R_{r,t}\,\partial_\tau(t)\right)}{R_r{}^2\, R} + \frac{\left(R\, R_{r,t} + 2\, R_r\, R_t\right)\partial_\tau(R)}{R_r\, R^2}\Bigg) = -8\,\pi\,\gamma_\mu{}^\beta\, \boldsymbol{n}^\tau\, \mathrm{T}_{\beta,\tau} \quad \mathbf{(89)}$$

> $TensorArray(eq_2, simplifier = simplify)$

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The second equation, $eq_2$, is identically satisfied

> $eq_2$

$$\mathcal{D}_{\beta}\left(\mathbf{K}_{\mu}{}^{\beta}\right) - \gamma_{\mu}{}^{\tau}\Bigg( -\frac{1}{R_r R}\Big(\partial_\tau(R)\, R_{r,t} + R\left(R_{r,r,t}\,\partial_\tau(r) + R_{r,t,t}\,\partial_\tau(t)\right) + 2\left(R_{r,r}\,\partial_\tau(r) + R_{r,t}\,\partial_\tau(t)\right) R_t + 2\,R_r\left(R_{r,t}\,\partial_\tau(r) + R_{t,t}\,\partial_\tau(t)\right)\Big) + \frac{\left(R\,R_{r,t} + 2\,R_r R_t\right)\left(R_{r,r}\,\partial_\tau(r) + R_{r,t}\,\partial_\tau(t)\right)}{R_r^{\,2}\,R} + \frac{\left(R\,R_{r,t} + 2\,R_r R_t\right)\partial_\tau(R)}{R_r R^2}\Bigg) = -8\,\pi\,\gamma_{\mu}{}^{\beta}\, \boldsymbol{n}^{\tau}\,\mathrm{T}_{\beta,\tau} \quad (89)$$

> $TensorArray\left(eq_2, simplifier = simplify\right)$

$$\left[\; 0=0 \quad 0=0 \quad 0=0 \quad 0=0 \;\right] \quad (90)$$

The fourth equation, $eq_4$, is also identically satisfied (basically, this is the definition of the ExtrinsicCurvature)

> $eq_4$

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$$\mathcal{D}_{\beta}\left(\mathrm{K}_{\mu}{}^{\beta}\right) - \gamma_{\mu}{}^{\tau}\Bigg( -\frac{1}{R_r R}\Big(\partial_\tau(R)\, R_{r,t} + R\left(R_{r,r,t}\,\partial_\tau(r) + R_{r,t,t}\,\partial_\tau(t)\right) + 2\left(R_{r,r}\,\partial_\tau(r) + R_{r,t}\,\partial_\tau(t)\right) R_t + 2\,R_r\left(R_{r,t}\,\partial_\tau(r) + R_{t,t}\,\partial_\tau(t)\right)\Big) + \frac{\left(R\,R_{r,t} + 2\,R_r R_t\right)\left(R_{r,r}\,\partial_\tau(r) + R_{r,t}\,\partial_\tau(t)\right)}{R_r{}^2\,R} + \frac{\left(R\,R_{r,t} + 2\,R_r R_t\right)\partial_\tau(R)}{R_r R^2}\Bigg) = -8\,\pi\,\gamma_{\mu}{}^{\beta}\, n^{\tau}\,\mathrm{T}_{\beta,\tau} \quad (89)$$

> $TensorArray(eq_2, simplifier = simplify)$

$$\left[\; 0=0 \quad 0=0 \quad 0=0 \quad 0=0 \;\right] \quad (90)$$

The fourth equation, $eq_4$, is also identically satisfied (basically, this is the definition of the ExtrinsicCurvature)

> $eq_4$

> $TensorArray(eq_2, simplifier = simplify)$

So it is in $eq_3$ where the evolution of the gravitational field is encoded, in terms of the functions $\{\rho_M, E(r), R(t, r)\}$ and their derivatives

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> $TensorArray(eq_2, simplifier = simplify)$

$$\left[\, 0=0 \quad 0=0 \quad 0=0 \quad 0=0 \,\right] \tag{90}$$

The fourth equation, $eq_4$, is also identically satisfied (basically, this is the definition of the ExtrinsicCurvature)

> $eq_4$

$$t^{\tau} \mathcal{D}_{\tau}\left(\gamma_{\mu,\nu}\right) + \gamma_{\nu,\tau} \mathcal{D}_{\mu}\left(t^{\tau}\right) + \gamma_{\mu,\tau} \mathcal{D}_{\nu}\left(t^{\tau}\right) = -2\, K_{\mu,\nu} + \beta^{\tau} \mathcal{D}_{\tau}\left(\gamma_{\mu,\nu}\right) + \gamma_{\nu,\tau} \mathcal{D}_{\mu}\left(\beta^{\tau}\right) + \gamma_{\mu,\tau} \mathcal{D}_{\nu}\left(\beta^{\tau}\right) \tag{91}$$

> $TensorArray(eq_2, simplifier = simplify)$

$$\left[\, 0=0 \quad 0=0 \quad 0=0 \quad 0=0 \,\right] \tag{92}$$

So it is in $eq_3$ where the evolution of the gravitational field is encoded, in terms of the functions $\{\rho_M, E(r), R(t, r)\}$ and their derivatives

> $eq_3$

> $EQ3 := TensorArray(eq_3, simplifier = simplify)$

To demonstrate that the system of equations $EQ3$ together with the constraint $eq_1$ is equivalent to the 4D system of equations $EQ4$ it now suffices to show that each of these two systems entirely reduces the other one. For this purpose, convert these arrays of equations to sets of equations

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$$\left[\ 0=0\ \ 0=0\ \ 0=0\ \ 0=0\ \right] \quad (90)$$

The fourth equation, $eq_4$, is also identically satisfied (basically, this is the definition of the ExtrinsicCurvature)

> $eq_4$

$$t^{\tau}\mathcal{D}_{\tau}\left(\gamma_{\mu,\nu}\right)+\gamma_{\nu,\tau}\mathcal{D}_{\mu}\left(t^{\tau}\right)+\gamma_{\mu,\tau}\mathcal{D}_{\nu}\left(t^{\tau}\right)=-2\,K_{\mu,\nu}+\beta^{\tau}\mathcal{D}_{\tau}\left(\gamma_{\mu,\nu}\right)+\gamma_{\nu,\tau}\mathcal{D}_{\mu}\left(\beta^{\tau}\right)+\gamma_{\mu,\tau}\mathcal{D}_{\nu}\left(\beta^{\tau}\right) \quad (91)$$

> $TensorArray(eq_2, simplifier = simplify)$

$$\left[\ 0=0\ \ 0=0\ \ 0=0\ \ 0=0\ \right] \quad (92)$$

So it is in $eq_3$ where the evolution of the gravitational field is encoded, in terms of the functions $\{\rho_M, E(r), R(t, r)\}$ and their derivatives

> $eq_3$

$$t^{\tau}\mathcal{D}_{\tau}\left(K_{\mu,\nu}\right)+K_{\nu,\tau}\mathcal{D}_{\mu}\left(t^{\tau}\right)+K_{\mu,\tau}\mathcal{D}_{\nu}\left(t^{\tau}\right)=-\frac{\left(R\,R_{r,t}+2\,R_r\,R_t\right)K_{\mu,\nu}}{R_r\,R}-2\,K_{\mu,\tau}K^{\tau}{}_{\nu}+R_{\mu,\nu}-8\,\pi\left(\gamma_{\mu}{}^{\kappa}\,\gamma_{\nu}{}^{\lambda}\,T_{\kappa,\lambda}-\frac{\gamma_{\mu,\nu}\left(\gamma_{\kappa}{}^{\lambda}\,\gamma^{\kappa,\sigma}\,T_{\lambda,\sigma}-T^{\alpha,\beta}\,n_{\alpha}\,n_{\beta}\right)}{2}\right)+\beta^{\tau}\mathcal{D}_{\tau}\left(K_{\mu,\nu}\right)+K_{\nu,\tau}\mathcal{D}_{\mu}\left(\beta^{\tau}\right)+K_{\mu,\tau}\mathcal{D}_{\nu}\left(\beta^{\tau}\right) \quad (93)$$

> $EQ3 := TensorArray(eq_3, simplifier = simplify)$

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$$\left[0 = 0, -R_t^2 - R\,R_{t,\,t} = \frac{R\,R_t\,R_{r,\,t} + \left(-4\,\pi\,\left(\rho_M + 2\,\rho_\Lambda\right)R^2 - 2\,E\right)R_r - R\,E_r}{R_r}, 0 = 0, 0 = 0\right]$$

$$\left[0 = 0, 0 = 0, \left(-R_t^2 - R\,R_{t,\,t}\right)\sin(\theta)^2 = -\frac{\left(-R\,R_t\,R_{r,\,t} + \left(4\,\pi\,\left(\rho_M + 2\,\rho_\Lambda\right)R^2 + 2\,E\right)R_r + R\,E_r\right)\sin(\theta)^2}{R_r}\right.$$

$$\left.0 = 0\right]$$

$$\left[0 = 0, 0 = 0, 0 = 0, 0 = 0\right]\Big]$$

To demonstrate that the system of equations *EQ3* together with the constraint $eq_1$ is equivalent to the 4D system of equations *EQ4* it now suffices to show that each of these two systems entirely reduces the other one. For this purpose, convert these arrays of equations to sets of equations

```
> EQ4 := convert(EQ4, setofequations)
```

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P. Fiziev, ***Withholding Potentials, Absence of Ghosts and Relationship between Minimal Dilatonic Gravity and f(R) Theories***, Phys. Rev. D 87, 044053 (2013)

Given the spacetime metric,

$$g_{\mu,\nu} = \begin{bmatrix} -e^{\lambda(r)} & 0 & 0 & 0 \\ 0 & -r^2 & 0 & 0 \\ 0 & 0 & -r^2 \sin(\theta)^2 & 0 \\ 0 & 0 & 0 & e^{\nu(r)} \end{bmatrix}$$

**a)** Compute the trace of

$$Z_{\alpha}^{\ \beta} = \Phi R_{\alpha}^{\ \beta} + \mathcal{D}_{\alpha} \mathcal{D}^{\beta} \Phi + T_{\alpha}^{\ \beta}$$

where $\Phi \equiv \Phi(r)$ is some function of the radial coordinate, $R_{\alpha}^{\ \beta}$ is the Ricci tensor, $\mathcal{D}_{\alpha}$ is the covariant derivative operator and $T_{\alpha}^{\ \beta}$ is the stress-energy tensor

$$\begin{bmatrix} 8\, e^{\lambda(r)} \pi & 0 & 0 & 0 \end{bmatrix}$$

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> *Setup*(*metric* = *ds2*) : *g_*[ ]

The indicated stress-energy tensor

> $T[\text{alpha}, \text{beta}] = 8 \cdot \text{Pi} \cdot \mathit{Matrix}(4, \langle \exp(\text{lambda}(r)), r^2, r^2 \sin(\text{theta})^2, \text{epsilon} \exp(\text{nu}(r)) \rangle, \mathit{shape} = \mathit{diagonal})$

> *Define*(??)

Solve item **a)** in one go, that is the trace of *Z*, defining the tensorial equation $Z_\alpha{}^\beta = \Phi\, R_\alpha{}^\beta + \mathscr{D}_\alpha \mathscr{D}^\beta \Phi + T_\alpha{}^\beta$

> *CompactDisplay*(Phi(*r*))

> $Z[\text{mu}, \text{nu}] = \text{Phi}(r)\ \mathit{Ricci}[\text{mu}, \text{nu}] + 'D\_[\text{mu}](D\_[\text{nu}](\text{Phi}(r)))' + T[\text{mu}, \text{nu}]$

> *Define*(??)

The answer to **a)**, that is the trace of $Z_{\mu, \nu}$

> *Z*[*trace*]

> *show*;

>

▶ *b) The components of* $W_\alpha{}^\beta \equiv$ *the traceless part of* $Z_\alpha{}^\beta$

▶ *c) An exact solution for the nonlinear system of differential equations conformed by the components of*

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The square of the line element and the metric

> $ds2 := \exp(\mathrm{nu}(r))dt^2 - \exp(\mathrm{lambda}(r))dr^2 - r^2\, dtheta^2 - r^2 \sin(\mathrm{theta})^2 dphi^2$

$$ds2 := \mathrm{e}^{\nu(r)}\, dt^2 - \mathrm{e}^{\lambda(r)}\, dr^2 - r^2\, d\theta^2 - r^2 \sin(\theta)^2\, d\phi^2 \quad (100)$$

> *CompactDisplay*(*ds2*)

*lambda*(*r*) *will now be displayed as* λ

*nu*(*r*) *will now be displayed as* ν (101)

> *Setup*(*metric* = *ds2*) : g_[ ]

$$g_{\mu,\nu} = \begin{bmatrix} -\mathrm{e}^{\lambda} & 0 & 0 & 0 \\ 0 & -r^2 & 0 & 0 \\ 0 & 0 & -r^2\sin(\theta)^2 & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\nu} \end{bmatrix} \quad (102)$$

The indicated stress-energy tensor

> $T[\mathrm{alpha}, \mathrm{beta}] = 8\cdot \mathrm{Pi}\cdot Matrix\left(4, \langle \exp(\mathrm{lambda}(r)), r^2, r^2 \sin(\mathrm{theta})^2, \mathrm{epsilon}\exp(\mathrm{nu}(r))\rangle, shape = diagonal\right)$

> *Define*( ?? )

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$$g_{\mu,\nu} = \begin{bmatrix} 0 & -r^2 & 0 & 0 \\ 0 & 0 & -r^2\sin(\theta)^2 & 0 \\ 0 & 0 & 0 & e^{\nu} \end{bmatrix} \quad \textbf{(102)}$$

The indicated stress-energy tensor

> $T[\text{alpha}, \text{beta}] = 8 \cdot \text{Pi} \cdot Matrix\left(4, \left\langle \exp(\text{lambda}(r)), r^2, r^2 \sin(\text{theta})^2, \text{epsilon} \exp(\text{nu}(r)) \right\rangle, shape = diagonal\right)$

$$T_{\alpha,\beta} = \begin{bmatrix} 8\pi e^{\lambda} & 0 & 0 & 0 \\ 0 & 8\pi r^2 & 0 & 0 \\ 0 & 0 & 8\pi r^2\sin(\theta)^2 & 0 \\ 0 & 0 & 0 & 8\pi\epsilon e^{\nu} \end{bmatrix} \quad \textbf{(103)}$$

> $Define(\textbf{(103)})$

Solve item **a)** in one go, that is the trace of $Z$, defining the tensorial equation $Z_{\alpha}{}^{\beta} = \Phi R_{\alpha}{}^{\beta} + \mathcal{D}_{\alpha} \mathcal{D}^{\beta} \Phi + T_{\alpha}{}^{\beta}$

> $CompactDisplay(\text{Phi}(r))$

> $Z[\text{mu}, \text{nu}] = \text{Phi}(r)\ Ricci[\text{mu}, \text{nu}] + 'D\_[\text{mu}](D\_[\text{nu}](\text{Phi}(r)))' + T[\text{mu}, \text{nu}]$

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> $T[\text{alpha}, \text{beta}] = 8 \cdot \text{Pi} \cdot Matrix\left(4, \langle \exp(\text{lambda}(r)), r^2, r^2 \sin(\text{theta})^2, \text{epsilon} \exp(\text{nu}(r)) \rangle, shape = diagonal\right)$

$$T_{\alpha, \beta} = \begin{bmatrix} 8\pi e^{\lambda} & 0 & 0 & 0 \\ 0 & 8\pi r^2 & 0 & 0 \\ 0 & 0 & 8\pi r^2 \sin(\theta)^2 & 0 \\ 0 & 0 & 0 & 8\pi \epsilon e^{\nu} \end{bmatrix} \quad (103)$$

> $Define(\mathbf{(103)})$

*Defined objects with tensor properties*

$$\left\{ \mathcal{D}_{\mu}, \gamma_{\mu}, \sigma_{\mu}, R_{\mu, \nu}, R_{\mu, \nu, \alpha, \beta}, T_{\alpha, \beta}, C_{\mu, \nu, \alpha, \beta}, X_{\mu}, \partial_{\mu}, g_{\mu, \nu}, \Gamma_{\mu, \nu, \alpha}, G_{\mu, \nu}, \delta_{\mu, \nu}, \epsilon_{\alpha, \beta, \mu, \nu} \right\} \quad (104)$$

Solve item **a)** in one go, that is the trace of $Z$, defining the tensorial equation $Z_{\alpha}^{\ \beta} = \Phi R_{\alpha}^{\ \beta} + \mathcal{D}_{\alpha} \mathcal{D}^{\beta} \Phi + T_{\alpha}^{\ \beta}$

> $CompactDisplay(\text{Phi}(r))$

> $Z[\text{mu}, \text{nu}] = \text{Phi}(r)\ Ricci[\text{mu}, \text{nu}] + 'D\_[\text{mu}](D\_[\text{nu}](\text{Phi}(r)))' + T[\text{mu}, \text{nu}]$

> $Define(\mathbf{??})$

The answer to **a)**, that is the trace of $Z_{\mu, \nu}$

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$$T_{\alpha, \beta} = \begin{bmatrix} 0 & 8\pi r & 0 & 0 \\ 0 & 0 & 8\pi r^2 \sin(\theta)^2 & 0 \\ 0 & 0 & 0 & 8\pi \epsilon e^{\nu} \end{bmatrix} \quad (103)$$

> $Define((103))$

*Defined objects with tensor properties*

$$\left\{ \mathcal{D}_{\mu}, \gamma_{\mu}, \sigma_{\mu}, R_{\mu, \nu}, R_{\mu, \nu, \alpha, \beta}, T_{\alpha, \beta}, C_{\mu, \nu, \alpha, \beta}, X_{\mu}, \partial_{\mu}, g_{\mu, \nu}, \Gamma_{\mu, \nu, \alpha}, G_{\mu, \nu}, \delta_{\mu, \nu}, \epsilon_{\alpha, \beta, \mu, \nu} \right\} \quad (104)$$

Solve item **a)** in one go, that is the trace of $Z$, defining the tensorial equation $Z_{\alpha}^{\beta} = \Phi R_{\alpha}^{\beta} + \mathcal{D}_{\alpha}\mathcal{D}^{\beta}\Phi + T_{\alpha}^{\beta}$

> $CompactDisplay(\mathrm{Phi}(r))$

*Phi(r) will now be displayed as* $\Phi$ (105)

> $Z[\mathrm{mu}, \mathrm{nu}] = \mathrm{Phi}(r)\ Ricci[\mathrm{mu}, \mathrm{nu}] + 'D\_[\mathrm{mu}](D\_[\mathrm{nu}](\mathrm{Phi}(r)))' + T[\mathrm{mu}, \mathrm{nu}]$

> $Define(??)$

The answer to **a)**, that is the trace of $Z_{\mu, \nu}$

> $Z[trace]$

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> $W[\text{mu},\sim\text{nu}, \mathit{matrix}]$

$$W_{\mu}^{\ \nu} = \left[\left[\frac{1}{8\,r^2}\left(\left(-6\,\Phi_{r,r}\,r^2 + 2\,\nu_{r,r}\,\Phi\,r^2 + \nu_r^{\,2}\,\Phi\,r^2 - r\left(\Phi\,\lambda_r\,r - r\,\Phi_r + 4\,\Phi\right)\nu_r + \left(3\,r^2\,\Phi_r - 4\,\Phi\,r\right)\lambda_r + 4\,r\,\Phi_r - 4\,\Phi\right)e^{-\lambda} + 4\,\Phi + \left(-16\,\epsilon - 16\right)\pi\,r^2\right), 0, 0, 0\right],\right.$$
$$\left[0, \frac{1}{8\,r^2}\left(\left(2\,\Phi_{r,r}\,r^2 - 2\,\nu_{r,r}\,\Phi\,r^2 + \left(r^2\,\nu_r - r^2\,\lambda_r - 4\,r\right)\Phi_r - \Phi\left(r^2\,\nu_r^{\,2} - r^2\,\nu_r\,\lambda_r - 4\right)\right)e^{-\lambda} - 4\,\Phi + \left(-16\,\epsilon - 16\right)\pi\,r^2\right), 0, 0\right],$$
$$\left[0, 0, \frac{1}{8\,r^2}\left(\left(2\,\Phi_{r,r}\,r^2 - 2\,\nu_{r,r}\,\Phi\,r^2 + \left(r^2\,\nu_r - r^2\,\lambda_r - 4\,r\right)\Phi_r - \Phi\left(r^2\,\nu_r^{\,2} - r^2\,\nu_r\,\lambda_r - 4\right)\right)e^{-\lambda} - 4\,\Phi + \left(-16\,\epsilon - 16\right)\pi\,r^2\right), 0\right],$$
$$\left.\left[0, 0, 0, \frac{1}{8\,r^2}\left(\left(2\,\Phi_{r,r}\,r^2 + 2\,\nu_{r,r}\,\Phi\,r^2 + \nu_r^{\,2}\,\Phi\,r^2 - r\left(\Phi\,\lambda_r\,r + 3\,r\,\Phi_r - 4\,\Phi\right)\nu_r + \left(-r^2\,\Phi_r + 4\,\Phi\,r\right)\lambda_r + 4\,r\,\Phi_r - 4\,\Phi\right)e^{-\lambda} + 4\,\Phi + \left(48\,\epsilon + 48\right)\pi\,r^2\right)\right]\right] \quad (111)$$

>

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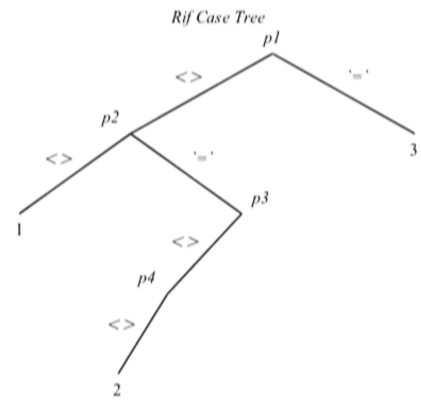
========== *Pivots Legend* ==========

$$p1 = -r\,\Phi_r + 2\,\Phi$$

$$p2 = r^2\,\Phi\left(\nu_r\,r - 2\right)\Phi_{r,r} - \left(\nu_{r,r}\,\Phi\,r^2 + \left(-r^2\,\nu_r + 2\,r\right)\Phi_r + \Phi\left(r^2\,\nu_r^2 - 2\right)\right)\left(r\,\Phi_r - 2\,\Phi\right)$$

$$p3 = \Phi + (12\,\epsilon + 12)\,r^2\,\pi$$

$$p4 = -12\left(\frac{\Phi}{12} + \pi\,r^2\,(\epsilon+1)\right)r\,\Phi_r + 2\,\Phi^2 + 28\,\pi\,r^2\,(\epsilon+1)\,\Phi + 32\,\pi^2\,r^4\,(\epsilon+1)^2$$




There are three cases

> *nops*(*Cases*)

$$3 \tag{113}$$

> $map(length, Cases)$

$$[5399, 1661, 405] \tag{114}$$

An exact solution for Cases[3]

> $sys[3] := op(1, Cases[3])$

$$sys_3 := \left[ e^{-\lambda} = -\frac{4\pi r^2 (\epsilon+1)}{\Phi}, \lambda_r = 0, \nu_{r,r} = \frac{-r^4 \pi (\epsilon+1) \nu_r^2 + 2 r^3 \pi (\epsilon+1) \nu_r + \Phi + (4\epsilon+4)\pi r^2}{2 r^4 \pi (\epsilon+1)}, \Phi_r = \frac{2\Phi}{r} \right] \tag{115}$$

> $constraint, subsystem := selectremove(has, sys[3], \exp)$

$$constraint, subsystem := \left[ e^{-\lambda} = -\frac{4\pi r^2 (\epsilon+1)}{\Phi} \right], \left[ \lambda_r = 0, \nu_{r,r} = \frac{-r^4 \pi (\epsilon+1) \nu_r^2 + 2 r^3 \pi (\epsilon+1) \nu_r + \Phi + (4\epsilon+4)\pi r^2}{2 r^4 \pi (\epsilon+1)}, \Phi_r = \frac{2\Phi}{r} \right] \tag{116}$$

> $sol_{subsystem} := dsolve(subsystem, explicit)$

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> $odetest(solution, ode_{system})$

$$\{0\} \qquad (121)$$

>

▶ General Relativity and Gravitation, Vol. 12, No. 9, (1980).

▶ Phys. Rev. A 74, 043405, (2006)

▼ Phys. Rev. D 51, 2713, (1995)

[1] E. Calzetta and C. El Hasi, ***Nontrivial dynamics in the early stages of inflation*** **Phys. Rev. D 51, 2713, (1995)**

The authors developed a perturbative study of the influence of the scalar radiation field on the expansion of the universe in the early stages of inflation. They performed numerical experiments to exhibit chaotic behavior indicated by the destruction of tori structures, formation of cantori, and Arnold diffusion.

>

▶ The Poincare surface-of-sections method

▶ The Hamiltonian and Poincare surface-of-sections of the paper

# ▶ The Physics Project and what's next

Maple Default Profile /Users/ecterrab/Maple/lib Server: 4 Memory: 85.72M Time: 31.18s Zoom: 300% Text Mode

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> $odetest(solution, ode_{system})$

$$\{0\} \quad (121)$$

>

▶ General Relativity and Gravitation, Vol. 12, No. 9, (1980).

▶ Phys. Rev. A 74, 043405, (2006)

▼ Phys. Rev. D 51, 2713, (1995)

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If another constant of motion involving p1 and q1 exists (then the system is integrable), it is possible to use it to express p1 = p1(q1), i.e., the intersection points will lie on a smooth curve. The enclosed area will be an integral invariant and, as time flows, these smooth curves will draw surfaces in the phase space.

- For weakly perturbed systems, these surfaces of solution curves of regular motion (KAM surfaces) continue to exist for most initial conditions, breaking their topology near resonances to form "islands" chains. Within these islands, the topology is broken again to other chains and so on. Generally speaking, the KAM surfaces isolate thin layers of stochasticity and, as the perturbation strength is increased, transitions between layers merge, and the KAM surfaces progressively disappear resulting in complete stochastic motion.
- In this manner, the plotting of the intersection points of the solution curves with a given 2D-plane (the surface-of-section) permits the study of the existence of non-obvious constants of motion (isolating integrals in the context of Hamilton-Jacobi theory), lo- cal stability, transition from ordered to stochastic motion, and many other interesting properties.
- We recall that no general procedure for determining the integrability of an arbitrary Hamiltonian system, or even the number of such isolating integrals, has yet been found. As a consequence, the plotting of these surfaces-of-section plays an important role not only in numerical studies, but also in checking the consistency of analytical results obtained using perturbative methods.

Example:

```
> restart; with(DEtools) :
```

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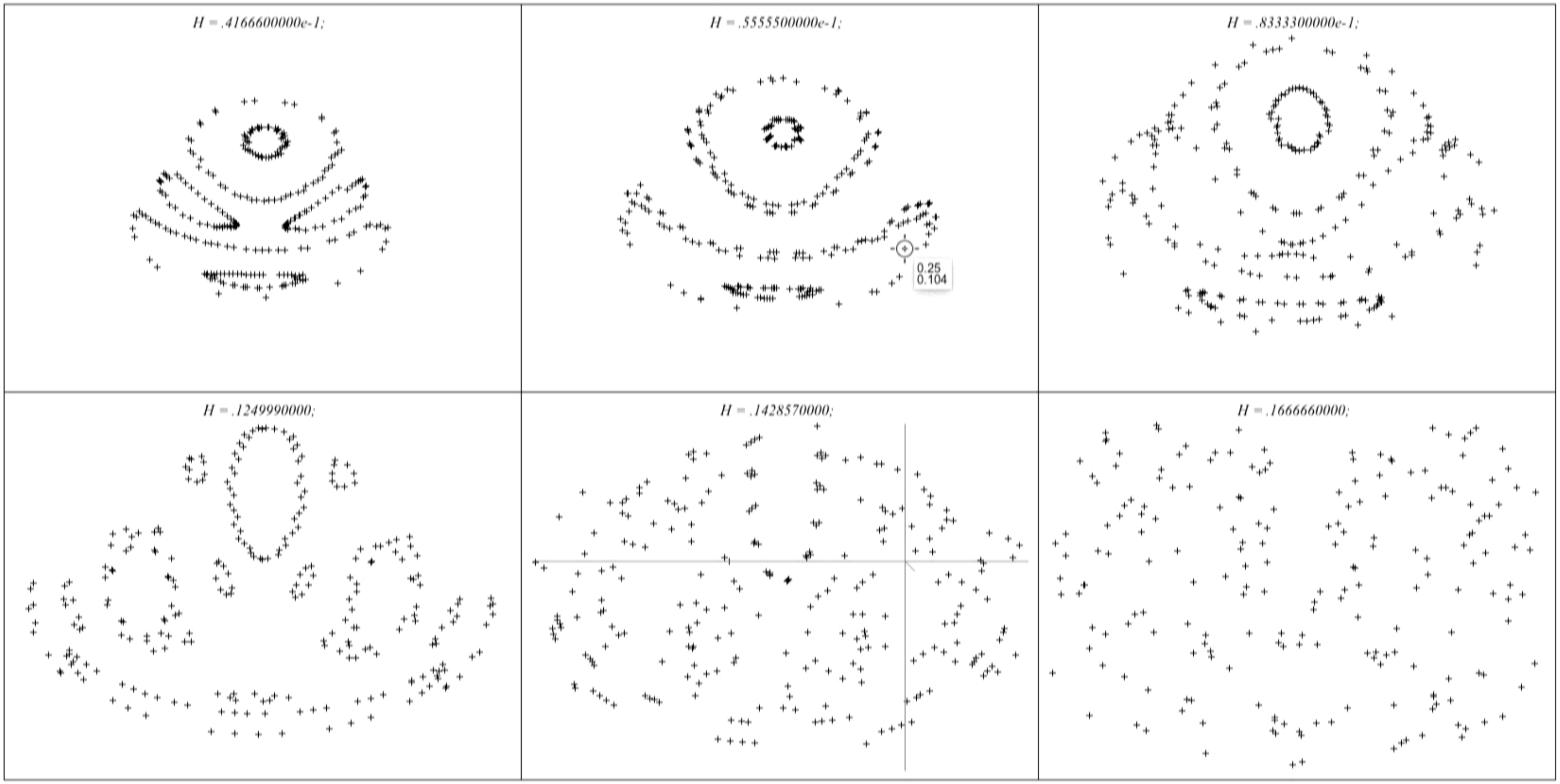
Draw the 6 Poincare surface of sections

> $plots[display]\left(Array\left(\left[\left[F4_{\frac{1}{24}}, F4_{\frac{1}{18}}, F4_{\frac{1}{12}}\right], \left[F4_{\frac{1}{8}}, F4_{\frac{1}{7}}, F4_{\frac{1}{6}}\right]\right]\right), axes = none\right)$




Maple Default Profile /Users/ecterrab/Maple/lib Server: 4 Memory: 23.19M Time: 34.26s Zoom: 300% Math Mode

Maple 2017 File Edit View Insert Format Table Drawing Plot Tools Window Help Tue Oct 24 10:59

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−0.7240000022, 0.7240000022, 0., 0.], [0., −0.7226666689, 0.7226666689, 0., 0.], [0.,
−0.7213333356, 0.7213333356, 0., 0.], [0., −0.7200000023, 0.7200000022, 0., 0.], [0.,
−0.7186666690, 0.7186666690, 0., 0.], [0., −0.7173333357, 0.7173333356, 0., 0.], [0.,
−0.7160000024, 0.7160000024, 0., 0.], [0., −0.7146666691, 0.7146666692, 0., 0.], [0.,
−0.7133333358, 0.7133333358, 0., 0.], [0., −0.7120000025, 0.7120000025, 0., 0.], [0.,
−0.7106666692, 0.7106666693, 0., 0.], [0., −0.7093333359, 0.7093333359, 0., 0.], [0.,
−0.7080000026, 0.7080000025, 0., 0.], [0., −0.7066666693, 0.7066666694, 0., 0.], [0.,
−0.7053333360, 0.7053333359, 0., 0.], [0., −0.7040000027, 0.7040000027, 0., 0.], [0.,
−0.7026666694, 0.7026666695, 0., 0.], [0., −0.7013333361, 0.7013333362, 0., 0.], [0.,
−0.7000000028, 0.7000000029, 0., 0.]}

> *ics* := *ic1* **union** *ic2* :

> *poincare*(*H*, *t* = 0 ..300, *ics*, *stepsize* = .1, *iterations* = 3, *scene* = [*q1* = −1.5 ..1.5, *p1* = −1 ..1, *q2* = −1 ..1], *quiet*)  # *17 seconds*

This figure is the one shown in the paper as Fig1-1. and shows the presence of smooth curves related to KAM surfaces, as well as a region of broken tori. More than 10,000 intersection points, absolute H-dev.≈10-8

It is interesting to see the plotting of a 3PS over (p1, q1, q2), for initial conditions very close to the critical point Pc

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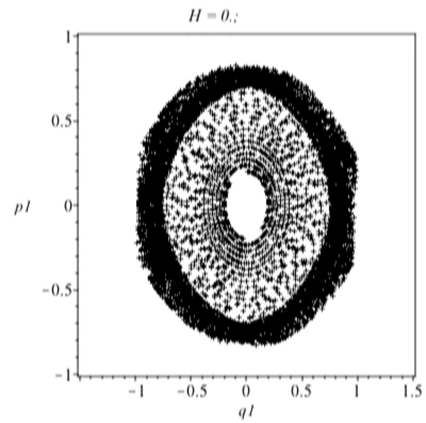
quiet)   # 17 seconds




This figure is the one shown in the paper as Fig1-1. and shows the presence of smooth curves related to KAM surfaces, as well as a region of broken tori. More than 10,000 intersection points, absolute H-dev.≈10-8

It is interesting to see the plotting of a 3PS over (p1, q1, q2), for initial conditions very close to the critical point Pc where p1 = p2 = q1 = q2 = 0:

```
> ics := generate_ic(H, {t = 0, p1 = 0 .. -0.31, q1 = 0, q2 = 0, energy = 0}, 40);
> P := poincare(H, t = 0 ..20, ics, stepsize = .1, scene = [q1 =-.3 ..0.3, p1 =-.3 ..0.3, q2 =-.1 ..0.1], 3, quiet) :
> plots[display](P, orientation = [-160, 50, 0], caption
      = `Fig. 1: Regular circles close to Pc, in agreement with complex eigenvalues for the linearized system`)
```

$-0.1271794883, 0.1271794883, 0., 0.], [0., -0.1192307704, 0.1192307704, 0., 0.], [0.,$
$-0.1112820525, 0.1112820525, 0., 0.], [0., -0.1033333346, 0.1033333346, 0., 0.], [0.,$
$-0.09538461665, 0.09538461664, 0., 0.], [0., -0.08743589870, 0.08743589869, 0., 0.], [0.,$
$-0.07948718075, 0.07948718075, 0., 0.], [0., -0.07153846280, 0.07153846280, 0., 0.], [0.,$
$-0.06358974485, 0.06358974485, 0., 0.], [0., -0.05564102690, 0.05564102690, 0., 0.], [0.,$
$-0.04769230895, 0.04769230894, 0., 0.], [0., -0.03974359100, 0.03974359101, 0., 0.], [0.,$
$-0.03179487305, 0.03179487305, 0., 0.], [0., -0.02384615510, 0.02384615510, 0., 0.], [0.,$
$-0.01589743715, 0.01589743715, 0., 0.], [0., -0.007948719201, 0.007948719201, 0., 0.], [0.,$
$-1.252\ 10^{-9}, 1.252000000\ 10^{-9}, 0., 0.]\}$

> $P := poincare(H, t = 0 ..20, ics, stepsize = .1, scene = [q1 = -.3 ..0.3, p1 = -.3 ..0.3, q2 = -.1 ..0.1], 3, quiet) :$

> *plots[display](P, orientation = [-160, 50, 0], caption = `Fig. 1: Regular circles close to Pc, in agreement with complex eigenvalues for the linearized system`)*

> *plots[display](P, orientation = [-20, 18, 0], caption = `Fig. 2: The action of higher order terms in splitting-up the KAM surfaces.`)*

>

# ▶ The Physics Project and what's next

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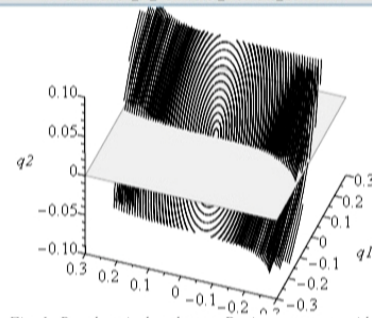


*Fig. 1: Regular circles close to Pc, in agreement with complex eigenvalues for the linearized system*

> $plots[display](P, orientation = [-20, 18, 0], caption = \text{`Fig. 2: The action of higher order terms in splitting-up the KAM surfaces.`})$

$H = 0.$;

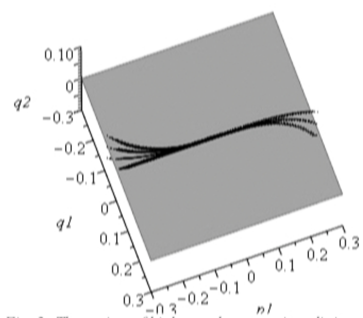


*Fig. 2: The action of higher order terms in splitting-up the KAM surfaces.*

>

# ▶ The Physics Project and what's next

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$$+ \ln(r) \left( \sqrt{(8\epsilon+8)\pi - \frac{\cdots}{e^{-\_C2}}} - 2\sqrt{\pi}(\epsilon+1) \right) \Bigg], \lambda = \_C2 \Bigg\}$$

Verifying this result

> $odetest(solution, ode_{system})$

$$\{0\} \tag{121}$$

>

# General Relativity and Gravitation, Vol. 12, No. 9, (1980).

A. Karlhede, ***A review of the geometrical equivalence of metrics in general relativity***, **General Relativity and Gravitation, Vol. 12, No. 9, (1980)**

## The example of the paper

## Generalization of the example of the paper:

>

# Phys. Rev. A 74, 043405, (2006)

# The Physics Project and what's next

*"Physics" is a software project at Maplesoft that started in 2006. The idea is to develop a computational symbolic/numeric environment specifically for Physics, targeting educational and research needs in equal footing, and resembling as much as possible the flexible style of computations used with paper and pencil. The main reference for the project is the Landau and Lifshitz Course of Theoretical Physics.*

*A first version of "Physics" with basic functionality appeared in 2007. Since then the package has been growing every year, including now, among other things, a searchable database of solutions to Einstein equations and a new dedicated programming language for Physics.*

*Since August/2013, weekly updates of the Physics package are distributed on the web, including the new developments related to our plan as well as related to people's feedback.*

## What's next ...

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▼ What's next ...

- ▶ The StandardModel subpackage ...
- ▶ The Scattering Matrix and Feynman Diagrams
- ▶ Numerical Relativity

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# What's next ...

## The StandardModel subpackage ...

Current restrictions: Not tested.

Aims at: allowing for the reproduction of the typical computations we do with the SM, as for instance shown in *The Standard Model, A Primer by Cliff by* Burgess and Moore.

**What we have in Maple 2017**

There are representations for all the fields of the SM, including implementation of SU gauge tensor indices and the Gell-Mann, Dirac and Pauli matrices and related algebra. The system also knows how to compute covariant differentiation taking into account gauge fields, possibly also spacetime curvature.

```
> with(Physics:-StandardModel)
>
```

## The Scattering Matrix and Feynman Diagrams

## Numerical Relativity

$HiggsBoson, Lagrangian, \Upsilon_{e}, \Upsilon_{\mu}, \Upsilon_{nu\_e}, \Upsilon_{nu\_mu}, \Upsilon_{nu\_tau}, \Upsilon_{\tau}, WeakField, WeakFieldStrength,$

$WeinbergAngle, q_{e}, q_{s}, q_{w}]$

\>

## The Scattering Matrix and Feynman Diagrams

Current restrictions:

- The Scattering matrix S is computed up to three vertices (products of up to three interaction Lagrangians)
- The drawing of the diagrams needs to be redesigned to work well for diagrams with more than one loop
- The computation of the Feynman integrals is not currently performed (they are only represented in the output); this is necessary in order to perform dimensional regularization and renormalization.

Aims at: allowing for computing perturbative expansions in field theory with no restrictions, including renormalization, first the standard computations shown in textbooks, then also numerical ones related to real experiments at CERN (collaboration with the European HiggsTools network).

**What we have in Maple 2017:**

\> $with(Physics)$ :

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**What we have in Maple 2017:**

> $with(Physics):$

> $Setup(mathematicalnotation = true)$

$$[mathematicalnotation = true] \tag{130}$$

> $Coordinates(X, Y, Z)$

*Default differentiation variables for d_, D_ and dAlembertian are:* $\{X = (x1, x2, x3, x4)\}$

*Systems of spacetime Coordinates are:* $\{X = (x1, x2, x3, x4), Y = (y1, y2, y3, y4), Z = (z1, z2, z3, z4)\}$

$$\{X, Y, Z\} \tag{131}$$

> $L := \lambda\, \phi(X)^4 + \sigma\, \eta(X)^3$

$$L := \lambda\, \phi(X)^4 + \sigma\, \eta(X)^3 \tag{132}$$

The expressions entering $S_1$ (only one vertex and so one evaluation point), representing the connected Feynman graphs for this interaction Lagrangian and discarding terms with tadpoles, is:

> $FeynmanDiagrams(L)$

$$\lambda\, :\phi(X)^4: + \sigma\, :\eta(X)^3: \tag{133}$$

> $FeynmanDiagrams(L, diagrams)$

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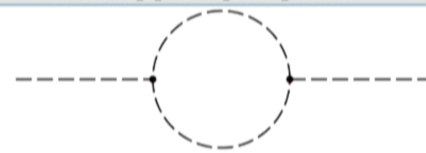
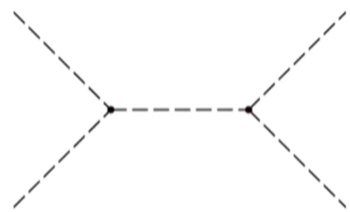


Symmetry factor = 18

$: \eta(X)^2\, \eta(Y)^2 : [\eta(X), \eta(Y)]$



Symmetry factor = 9

$$16\,\lambda^2 : \phi(X)^3\, \phi(Y)^3 : [\phi(X), \phi(Y)] + 96\,\lambda^2 : \phi(X)\, \phi(Y) : [\phi(X), \phi(Y)]^3 + 72\,\lambda^2 : \phi(X)^2\, \phi(Y)^2\, [\phi(X), \phi(Y)]^2 + 18\,\sigma^2 : \eta(X)\, \eta(Y) : [\eta(X), \eta(Y)]^2 + 9\,\sigma^2 : \eta(X)^2\, \eta(Y)^2 : [\eta(X), \eta(Y)] \qquad (137)$$

>

## Numerical Relativity

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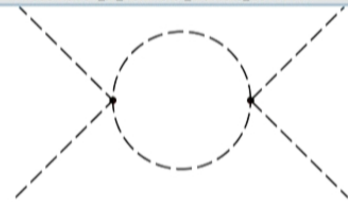
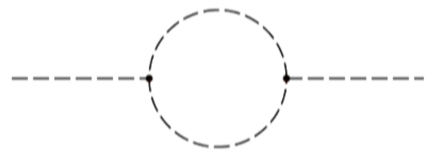


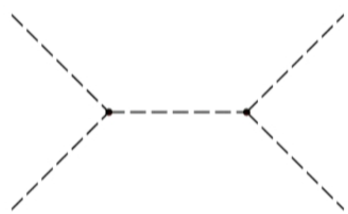
Symmetry factor = 72

$: \eta(X)\, \eta(Y) :\, [\eta(X), \eta(Y)]^2$



Symmetry factor = 18

$: \eta(X)^2\, \eta(Y)^2 :\, [\eta(X), \eta(Y)]$



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*check_parameters*, *check_shared_par*, *check_variables*, *chk_init*, *create_par_file*, *discr_rec*, *find_IC_rec*, *find_diff*, *find_var*, *find_vars_list*, *group_names*, *initial_wave3d*, *initial_wave3d_par*, *list_files*, *mc_all*, *mc_fun*, *ord_sched*, *par_names*, *quot*, *set_cactus_dir*, *set_thorn_IC*, *set_thorn_boundary*, *set_thorn_config*, *set_thorn_coords*, *set_thorn_descr*, *set_thorn_eqs*, *set_thorn_friend*, *set_thorn_implementation*, *set_thorn_inherits*, *set_thorn_init_sym*, *set_thorn_name*, *set_thorn_parameters*, *set_thorn_variables*, *var_names*, *write_banner*, *write_boundary*, *write_eq*, *write_interface*, *write_makedfn*, *write_par_file*, *write_param*, *write_schedule*, *write_sym*, *write_template*, *write_thorn*]

Set the directory where your thorn will be saved (you can set this directly to "~/Cactus/arrangements", or to a test folder (my choice):

> *set_cactus_dir*("/Users/ecterrab/Maple/extdev/lib/Physics/Cactus/output/")

"Setting current dir to: /Users/ecterrab/Maple/extdev/lib/Physics/Cactus/output/arrangements" **(139)**

Set the name of the thorn (i.e. the name of the directory where it will written)

> *Cactus*:-*set_thorn_name*("WaveToyTest")

"Warning, a thorn with such name already exists. If you continue, you'll overwrite the existing files."

"WaveToyTest" **(140)**

Set the name of the implementation:

> *set_thorn_implementation*("wavetoy")

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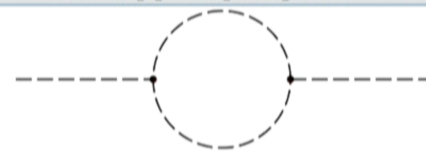
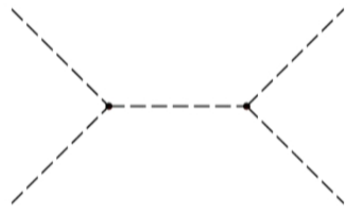


Symmetry factor = 18

$: \eta(X)^2 \, \eta(Y)^2 : [\eta(X), \eta(Y)]$



Symmetry factor = 9

$$16\,\lambda^2 \; : \phi(X)^3 \, \phi(Y)^3 : \, [\phi(X), \phi(Y)] + 96\,\lambda^2 \; : \phi(X) \, \phi(Y) : \, [\phi(X), \phi(Y)]^3 + 72\,\lambda^2 \; : \phi(X)^2 \, \phi(Y)^2 \, [\phi(X), \phi(Y)]^2 + 18\,\sigma^2 \; : \eta(X) \, \eta(Y) : \, [\eta(X), \eta(Y)]^2 + 9\,\sigma^2 \; : \eta(X)^2 \, \eta(Y)^2 : \, [\eta(X), \eta(Y)] \qquad (137)$$

>

# ▶ Numerical Relativity

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>

# Numerical Relativity

Current restrictions: under development

Aims at:

- Allowing for performing the typical computations of numerical relativity textbooks like "Baumgarte, T.W., Shapiro, S.L., Numerical Relativity, Solving Einstein's Equations on a Computer, Cambridge University Press, 2010. (The Physics and the ThreePlusOne package already covers up to Chapter 3)
- Allowing for running simulations in CACTUS (the Einstein Toolkit) directly from a Maple worksheet, departing from basic human-readable mathematical objects like a metric and a gauge choice for the Shift and Lapse, and initial conditions.

**What we have in the Maple Research version under development**

Convert the 3d scalar wave equation to a Cactus thorn, setting up all the necessary quantities and creating all the thorn files.

> *restart* :

> Cactus:-set_thorn_name("WaveToyTest")

"Warning, a thorn with such name already exists. If you continue, you'll overwrite the existing files."

"WaveToyTest" **(140)**

Set the name of the implementation:

> *set_thorn_implementation*("wavetoy")

"Other thorns with the same implementation:", *check_implementation*("wavetoy")

"wavetoy" **(141)**

This thorn inherits only the grid thorn and is friend with no other thorn.

> *set_thorn_inherits*([*grid*])

"The thorn inherits the following variables from implementation", *grid*, ":", *grid*

[*grid*] **(142)**

> *set_thorn_friend*( )

We use the default coordinates:

> *set_thorn_coords*( )

To set initial conditions for a PDE:

> *set_thorn_IC*( )

> *set_thorn_IC*([*wave3d*, "plane"])

Maple Default Profile /Users/ecterrab/Maple/extdev/lib/Physics/Cactus/output/arrangements Server: 4 Memory: 89.21M Time: 51.1s Zoom: 300% Math Mode

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[*grid*] **(142)**

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[ ] **(143)**

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$[t, x, y, z]$ **(144)**

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Maple Default Profile /Users/ecterrab/Maple/extdev/lib/Physics/Cactus/output/arrangements Server: 4 Memory: 89.21M Time: 51.1s Zoom: 300% Math Mode

$[\,]$ **(143)**

We use the default coordinates:

> *set_thorn_coords*( )

$[t, x, y, z]$ **(144)**

To set initial conditions for a PDE:

> *set_thorn_IC*( )

"To choose one of the 3d wave innial conditions, please use [wave3d, type], where type="plane", "gaussian", "box", or "none". "

"Custom ICs still not implemented, no ICs set" **(145)**

> *set_thorn_IC*( [ *wave3d*, "plane" ] )

"To choose one of the 3d wave innial conditions, please use [wave3d, type], where type="plane", "gaussian", "box", or "none". "

"ICs set to Wave3d", "plane" **(146)**

The parameter list should be in the form : [[par_name::type1, type2, [[Range1], Default_value], Descr]]): where TYPE1=[integer, real, keyword, boolean, string], TYPE2=[Global,Restricted, Private, shares::name_of_impl]

Note: here if one sets real parameter, then the default values should be written as float otherwise it gives error

> *set_thorn_parameters*( [ [ *bound*::*keyword*, *Restricted*, [ [ "none", "flat", "static", "radiation", "robin", "zero" ],

"To choose one of the 3d wave innial conditions, please use [wave3d, type], where type="plane", "gaussian", "box", or "none". "

"Custom ICs still not implemented, no ICs set" **(145)**

> *set_thorn_IC*([*wave3d*, "plane"])

"To choose one of the 3d wave innial conditions, please use [wave3d, type], where type="plane", "gaussian", "box", or "none". "

"ICs set to Wave3d", "plane" **(146)**

The parameter list should be in the form : [[par_name::type1, type2, [[Range1], Default_value], Descr]]): where TYPE1=[integer, real, keyword, boolean, string], TYPE2=[Global,Restricted, Private, shares::name_of_impl]

Note: here if one sets real parameter, then the default values should be written as float otherwise it gives error

> *set_thorn_parameters*([[*bound*::*keyword*, *Restricted*, [["none", "flat", "static", "radiation", "robin", "zero"], "none"], "Type of boundary condition to use"]])

[[*bound*::*keyword*, *Restricted*, [["none", "flat", "static", "radiation", "robin", "zero"], "none"], "Type of boundary condition to use"]] **(147)**

We can set a symmetry for the initial conditions (this following the Cactus documentation means choosing whether phi (x)=phi(-x) ->1, or phi(x)=-phi(-x)->-1):

> *set_thorn_init_sym*([$\phi$, [$-1$, 1, 1]])

> *set_thorn_IC*([*wave3d*, "plane"])

"To choose one of the 3d wave innial conditions, please use [wave3d, type], where type="plane", "gaussian", "box", or "none". "

"ICs set to Wave3d", "plane" **(146)**

The parameter list should be in the form : [[par_name::type1, type2, [[Range1], Default_value], Descr]]): where TYPE1=[integer, real, keyword, boolean, string], TYPE2=[Global,Restricted, Private, shares::name_of_impl]

Note: here if one sets real parameter, then the default values should be written as float otherwise it gives error

> *set_thorn_parameters*([[*bound*::*keyword*, *Restricted*, [["none", "flat", "static", "radiation", "robin", "zero"], "none"], "Type of boundary condition to use"]])

[[*bound*::*keyword*, *Restricted*, [["none", "flat", "static", "radiation", "robin", "zero"], "none"], "Type of boundary condition to use"]] **(147)**

We can set a symmetry for the initial conditions (this following the Cactus documentation means choosing whether phi (x)=phi(-x) ->1, or phi(x)=-phi(-x)->-1):

> *set_thorn_init_sym*([$\phi$, [ − 1, 1, 1]])

$$[\phi, [-1, 1, 1]]$$ **(148)**

We can also set boundary conditions from a predefined set:

> *set_thorn_boundary*($\phi$)

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fin_diff=(forward,central,backward) for example:

> #set_thorn_eqs(["evol_wave",Eq_wave, "at BASEGRID"], fin_diff=forward)

The list of thorn equations as Maple equations:

> *_m_thorn_eqs*

$$\left[\left[\left[\frac{\partial^2}{\partial x^2}\phi(t,x,y,z)+\frac{\partial^2}{\partial y^2}\phi(t,x,y,z)+\frac{\partial^2}{\partial z^2}\phi(t,x,y,z)=\frac{\partial^2}{\partial t^2}\phi(t,x,y,z)\right],\text{"central"},\text{"at EVOL"},\text{"evol\_wave"}\right]\right] \tag{154}$$

To set a description of the thorn:

> *set_thorn_descr*("This thorn solves the 3d wave equation.")

"This thorn solves the 3d wave equation." **(155)**

To write the thorn:

> *write_thorn*( )

"Changing dir to arrangements", "/Users/ecterrab/Maple/extdev/lib/Physics/Cactus/output/arrangements"

"Error, thorn already exists" **(156)**

To write a simple .par file use this: (it will be expanded when we start using the parameters DB).

> *write_par_file*( )

Maple Default Profile /Users/ecterrab/Maple/extdev/lib/Physics/Cactus/output/arrangements Server: 4 Memory: 55.19M Time: 52.29s Zoom: 300% Math Mode