COMPUTER ALGEBRA FOR THEORETICAL PHYSICS

Generally speaking, physicists still experience that computing with paper and pencil is in most cases simpler than computing on a Computer Algebra worksheet. On the other hand, recent developments in the Maple system implemented most of the mathematical objects and mathematics used in theoretical physics computations, and dramatically approximated the notation used in the computer to the one used in paper and pencil, diminishing the learning gap and computer-syntax distraction to a strict minimum. In connection, in this talk the Physics project at Maplesoft is presented and the resulting Physics package illustrated tackling problems in classical and quantum mechanics, general relativity and field theory. In addition to the 10 a.m lecture, there will be a hands-on workshop at 1pm in the Alice Room.

... Why computers?

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

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,

functional differentiation, relativity differential operators and sum rule for tensor contracted (repeated) indices

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

ability to move from inert to active representations of computations and viceversa as necessary

hand-like style for entering computations and texbook-like notation for displaying results

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

ability to handle products and derivatives involving commutative, anticommutative and noncommutative variables and functions

ability to perform computations taking into account custom-defined algebra rules of different kinds

(problem related commutator, anticommutator, bracket, etc. rules)

▼ Vector and tensor notation in mechanics, electrodynamics and relativity

Formalism	Formulation	Homogeneous equations	Non-homogeneous equations
Vector calculus	Fields 3D Euclidean space + time	$\nabla \cdot \mathbf{B} = 0$ $\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0$	$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$ $\nabla \times \mathbf{B} - \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J}$
	Potentials (any gauge) 3D Euclidean space + time	$\mathbf{B} = \nabla \times \mathbf{A}$ $\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}$	$\nabla^2\varphi + \frac{\partial}{\partial t}(\nabla \cdot \mathbf{A}) = -\frac{\rho}{\varepsilon_0}$ $\Box\mathbf{A} + \nabla\left(\nabla \cdot \mathbf{A} + \frac{1}{c^2}\frac{\partial \varphi}{\partial t}\right) = \mu_0 \mathbf{J}$
	Potentials (Lorenz gauge) 3D Euclidean space + time	$\mathbf{B} = \nabla \times \mathbf{A}$ $\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}$ $\nabla \cdot \mathbf{A} + \frac{1}{c^2}\frac{\partial \varphi}{\partial t} = 0$	$\Box\varphi = \frac{\rho}{\varepsilon_0}$ $\Box\mathbf{A} = \mu_0 \mathbf{J}$
Tensor calculus	Fields Minkowski space	$\partial_{[\alpha} F_{\beta\gamma]} = 0$	$\partial_\alpha F^{\beta\alpha} = \mu_0 J^\beta$
	Potentials (any gauge) Minkowski space	$F_{\alpha\beta} = \partial_{[\alpha} A_{\beta]}$	$\partial_\alpha \partial^{[\beta} A^{\alpha]} = \mu_0 J^\beta$
	Potentials (Lorenz gauge) Minkowski space	$F_{\alpha\beta} = \partial_{[\alpha} A_{\beta]}$ $\partial_\alpha A^\alpha = 0$	$\Box A^\alpha = -\mu_0 J^\alpha$
	Fields any space-time	$\partial_{[\alpha} F_{\beta\gamma]} = \nabla_{[\alpha} F_{\beta\gamma]} = 0$	$\nabla_\alpha(\sqrt{-g} F^{\beta\alpha}) = \mu_0 J^\beta$
	Potentials (any gauge) any space-time	$F_{\alpha\beta} = \partial_{[\alpha} A_{\beta]} = \nabla_{[\alpha} A_{\beta]}$	$\nabla_\alpha(\sqrt{-g}\nabla^{[\beta} A^{\alpha]}) = \mu_0 J^\beta$
	Potentials (Lorenz gauge) any space-time	$F_{\alpha\beta} = \partial_{[\alpha} A_{\beta]} = \nabla_{[\alpha} A_{\beta]}$, $\nabla_\alpha A^\alpha = 0$	$\Box A^\alpha - R^\alpha{}_\beta A^\beta = -\mu_0 J^\alpha$

Dirac's notation in quantum mechanics

$$|\Psi\rangle = \int |x\rangle\langle x|\Psi\rangle dx \qquad \langle\Phi| = \int \langle\Phi|x'\rangle\langle x'| dx'$$

$$\langle\Phi|\Psi\rangle = \int \langle\Phi|x\rangle\langle x|\Psi\rangle dx = \int \Phi^*(x)\Psi(x) dx$$

$$\langle E \rangle = \sum \langle \Phi | n \rangle E_n \langle n | \Phi \rangle = \sum_n |c_n|^2 E_n$$

$$\langle p | \Psi \rangle = \Psi(p) = \frac{1}{\sqrt{2\pi}} \int_0^1 \exp(-ipx) \sqrt{2} \sin(n\pi x) dx$$

- Computer algebra systems were not originally designed to work with this compact notation, having attached so dense mathematical contents, active and inert representations of operations, not commutative and customizable *algebraic* computational domain, and the related mathematical methods, all this typically present in computations in theoretical physics.
- This situation has changed. The notation and related mathematical methods are now implemented.

Tackling examples with the Physics package

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

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

$$InertiaTensor := \sum_{k=1}^{N} m_k \left(\left\|\vec{r}_k\right\|^2 \delta_{i,j} - \left(\vec{r}_k\right)_i \left(\vec{r}_k\right)_j \right) \tag{3.1.1.1.1}$$

There are 3 particles

> $N := 3$

$$N := 3 \tag{3.1.1.1.2}$$

Create an indexing function

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

$$IT := (i,j) \mapsto \sum_{k=1}^{3} m_k \left(\left\|\vec{r}_k\right\|^2 \delta_{i,j} - \left(\vec{r}_k\right)_i \left(\vec{r}_k\right)_j \right) \tag{3.1.1.1.3}$$

The inerta tensor matrix

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

$$IT\_Matrix := \left[\left[\sum_{k=1}^{3} m_k \left(\left\|\vec{r}_k\right\|^2 - \left(\vec{r}_k\right)_1^{\,2}\right), \sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_1 \left(\vec{r}_k\right)_2\right), \sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_1 \left(\vec{r}_k\right)_3\right)\right], \left[\sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_1 \left(\vec{r}_k\right)_2\right), \sum_{k=1}^{3} m_k \left(\left\|\vec{r}_k\right\|^2 - \left(\vec{r}_k\right)_2^{\,2}\right), \sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_2 \left(\vec{r}_k\right)_3\right)\right], \left[\sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_1 \left(\vec{r}_k\right)_3\right), \sum_{k=1}^{3} \left(-m_k \left(\vec{r}_k\right)_2 \left(\vec{r}_k\right)_3\right), \sum_{k=1}^{3} m_k \left(\left\|\vec{r}_k\right\|^2 - \left(\vec{r}_k\right)_3^{\,2}\right)\right]\right] \tag{3.1.1.1.4}$$

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

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

$$position := \vec{r}_k = \vec{R}_k - \vec{R}_{CM} \tag{3.1.1.1.5}$$

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

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

$$\vec{R}_1 := -\frac{a\,\hat{i}}{2} \quad (3.1.1.1.6)$$

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

$$\vec{R}_2 := h\,\hat{k} \quad (3.1.1.1.7)$$

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

$$\vec{R}_3 := \frac{a\,\hat{i}}{2} \quad (3.1.1.1.8)$$

Two masses are equal

> $m_3 := m[1]$

$$m_3 := m_1 \quad (3.1.1.1.9)$$

The "*center of mass*"

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

$$\vec{R}_{CM} := \frac{\sum_{j=1}^{3} m_j\,\vec{R}_j}{\sum_{j=1}^{3} m_j} \quad (3.1.1.1.10)$$

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

$$\vec{R}_{CM} := \frac{m_2\,h\,\hat{k}}{2\,m_1 + m_2} \quad (3.1.1.1.11)$$

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

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

$$\vec{r}_1 = -\frac{a\,\hat{i}}{2} - \frac{m_2\,h\,\hat{k}}{2\,m_1 + m_2}, \vec{r}_2 = h\,\hat{k} - \frac{m_2\,h\,\hat{k}}{2\,m_1 + m_2}, \vec{r}_3 = \frac{a\,\hat{i}}{2} - \frac{m_2\,h\,\hat{k}}{2\,m_1 + m_2} \quad (3.1.1.1.12)$$

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

> $IT\_answer := simplify(eval(value(IT\_Matrix), [\textbf{(3.1.1.1.12)}]))$

$$IT\_answer := \begin{bmatrix} \frac{2\, m_2\, h^2\, m_1}{2\, m_1 + m_2} & 0 & 0 \\ 0 & \frac{m_1\,(2\, m_1\, a^2 + a^2\, m_2 + 4\, m_2\, h^2)}{2\,(2\, m_1 + m_2)} & 0 \\ 0 & 0 & \frac{m_1\, a^2}{2} \end{bmatrix} \quad \textbf{(3.1.1.1.13)}$$

>

Quantum mechanics

Quantization of the energy of a particle in a magnetic field

Show that the energy of a particle in a constant magnetic field oriented along the z axis can be written as

$$H = \hbar\, \omega_c \left(a^{\dagger} a + \frac{1}{2}\right)$$

where $a^{\dagger}$ and a are creation and anihilation operators.

Solution

The classical Hamiltonian is given by

$$H = \frac{\left(\vec{p} - \frac{q\, \vec{A}}{c}\right)^2}{2\, m}$$

The underlying quantum mechanics algebra rules are

$$[(\vec{r})_i, (\vec{p})_j]_- = \delta_{i,j}, \quad [(\vec{r})_i, (\vec{r})_j]_- = 0, \quad [(\vec{p})_i, (\vec{p})_j]_- = 0$$

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

> $Setup\Big(hermitianoperators = \{\vec{A}, H, \Pi, \vec{\Pi}, p, \vec{p}, x, y, z\},\ quantumoperators = \{a\},$

$realobjects = \{\hbar, B, c, k, m, q, \omega_c\});$

$$\left[hermitianoperators = \{\vec{A}, H, \Pi, \vec{\Pi}, p, \vec{p}, x, y, z\}, quantumoperators = \{\vec{A}, H, \Pi, \vec{\Pi}, a, p, \vec{p}, x, y, z\}, realobjects = \{\hbar, B, \hat{i}, \hat{j}, \hat{k}, \hat{\phi}, \hat{r}, \hat{\rho}, \hat{\theta}, c, k, m, \phi, q, r, \rho, \theta, x, y, z, \omega_c\}\right] \quad (3.2.1.1.1)$$

The Hamiltonian

$> H = \frac{\vec{\Pi}^2}{2\ m}$

$$H = \frac{\vec{\Pi}^2}{2\,m} \quad (3.2.1.1.2)$$

where

$> \vec{\Pi} = p\_ - \frac{q}{c} \cdot A\_(x, y)$

$$\vec{\Pi} = \vec{p} - \frac{q\,\vec{A}(x, y)}{c} \quad (3.2.1.1.3)$$

$> PDEtools\text{:-}declare(A\_(x, y))$

$$\vec{A}(x, y) \textit{ will now be displayed as } \vec{A} \quad (3.2.1.1.4)$$

$> Setup(\{[x, p_x]_- = i\,\hbar, [x, p_y]_- = 0, [y, x]_- = 0, [y, p_x]_- = 0, [y, p_y]_- = i\,\hbar, [p_y, p_x]_- = 0\})$

$$\left[algebrarules = \{[x, p_x]_- = \mathrm{i}\,\hbar, [x, p_y]_- = 0, [y, x]_- = 0, [y, p_x]_- = 0, [y, p_y]_- = \mathrm{i}\,\hbar, [p_y, p_x]_- = 0\}\right] \quad (3.2.1.1.5)$$

In Coulomb's gauge, the following vector potential gives the magnetic field of the problem, $\vec{B} = B\,\hat{k}$

$> A\_(x, y) = -\frac{B \cdot y}{2} \cdot \_i + \frac{B \cdot x}{2} \cdot \_j;$

$$\vec{A} = -\frac{1}{2}\,B\,\hat{i}\,y + \frac{1}{2}\,B\,\hat{j}\,x \quad (3.2.1.1.6)$$

Indeed we have

$> Divergence(\textbf{(3.2.1.1.6)})$

$$\nabla \cdot \vec{A} = 0 \quad (3.2.1.1.7)$$

> $Curl((3.2.1.1.6))$

$$\nabla \times \vec{A} = B\,\hat{k} \tag{3.2.1.1.8}$$

Derive now the commutation rule for $[\Pi_x, \Pi_y]_-$

> $\vec{\Pi} = \Pi[x]\cdot\_i + \Pi[y]\cdot\_j;$

$$\vec{\Pi} = \hat{i}\,\Pi_x + \hat{j}\,\Pi_y \tag{3.2.1.1.9}$$

> $p\_ = p[x]\cdot\_i + p[y]\cdot\_j$

$$\vec{p} = \hat{i}\,p_x + \hat{j}\,p_y \tag{3.2.1.1.10}$$

> $subs((3.2.1.1.6), (3.2.1.1.9), (3.2.1.1.10), (3.2.1.1.3))$

$$\hat{i}\,\Pi_x + \hat{j}\,\Pi_y = \hat{i}\,p_x + \hat{j}\,p_y - \frac{q\left(-\frac{1}{2}\,B\,\hat{i}\,y + \frac{1}{2}\,B\,\hat{j}\,x\right)}{c} \tag{3.2.1.1.11}$$

> $Component((3.2.1.1.11), 1)$

$$\Pi_x = p_x + \frac{q\,B\,y}{2\,c} \tag{3.2.1.1.12}$$

> $Component((3.2.1.1.11), 2)$

$$\Pi_y = p_y - \frac{q\,B\,x}{2\,c} \tag{3.2.1.1.13}$$

> $Commutator((3.2.1.1.12), (3.2.1.1.13))$

$$[\Pi_x, \Pi_y]_- = \frac{\mathrm{i}\,q\,B\,\hbar}{c} \tag{3.2.1.1.14}$$

> $Setup((3.2.1.1.14))$

$$\left[algebrarules = \left\{[x, p_x]_- = \mathrm{i}\,\hbar,\ [x, p_y]_- = 0,\ [y, x]_- = 0,\ [y, p_x]_- = 0,\ [y, p_y]_- = \mathrm{i}\,\hbar,\ [\Pi_x, \Pi_y]_- = \frac{\mathrm{i}\,q\,B\,\hbar}{c},\ [p_y, p_x]_- = 0\right\}\right] \tag{3.2.1.1.15}$$

Time to bring in annihilation and creation operators

> $a = \frac{\sqrt{c}}{\sqrt{2\cdot\hbar\cdot q\cdot B}}\left(\Pi_x + \mathrm{i}\cdot\Pi_y\right)$

$$a = \frac{\sqrt{c}\,\sqrt{2}\,\left(\Pi_x + \mathrm{i}\,\Pi_y\right)}{2\,\sqrt{\hbar\,q\,B}} \tag{3.2.1.1.16}$$

> $(3.2.1.1.16)^*$

$$a^{\dagger} = \frac{\sqrt{c}\,\sqrt{2}\,\left(\Pi_x - \mathrm{i}\,\Pi_y\right)}{2\,\sqrt{\hbar\,q\,B}} \tag{3.2.1.1.17}$$

Verify the normalization of this definition

> *Commutator*((**3.2.1.1.16**), (**3.2.1.1.17**))

$$\left[a, a^{\dagger}\right]_{-} = 1 \tag{3.2.1.1.18}$$

> *Setup*((**3.2.1.1.18**))

$$\left[algebrarules = \left\{\left[a, a^{\dagger}\right]_{-} = 1, \left[x, p_x\right]_{-} = \mathrm{i}\,\hbar, \left[x, p_y\right]_{-} = 0, \left[y, x\right]_{-} = 0, \left[y, p_x\right]_{-} = 0, \left[y, p_y\right]_{-} = \mathrm{i}\,\hbar, \left[\Pi_x, \Pi_y\right]_{-} = \frac{\mathrm{i}\,q\,B\,\hbar}{c}, \left[p_y, p_x\right]_{-} = 0\right\}\right] \tag{3.2.1.1.19}$$

To express the Hamiltonian in terms of a, $a^{\dagger}$

> *subs*((**3.2.1.1.9**), (**3.2.1.1.2**))

$$H = \frac{\left(\hat{i}\,\Pi_x + \hat{j}\,\Pi_y\right)^2}{2\,m} \tag{3.2.1.1.20}$$

> *solve*({(**3.2.1.1.16**), (**3.2.1.1.17**)}, $\{\Pi_x, \Pi_y\}$)

$$\left\{\Pi_x = \frac{\sqrt{\hbar\,q\,B}\,\left(a^{\dagger} + a\right)\sqrt{2}}{2\,\sqrt{c}}, \Pi_y = \frac{\frac{\mathrm{i}}{2}\,\sqrt{\hbar\,q\,B}\,\left(a^{\dagger} - a\right)\sqrt{2}}{\sqrt{c}}\right\} \tag{3.2.1.1.21}$$

> *subs*((**3.2.1.1.21**), (**3.2.1.1.20**))

$$H = \frac{\left(\frac{\hat{i}\,\sqrt{\hbar\,q\,B}\,\left(a^{\dagger} + a\right)\sqrt{2}}{2\,\sqrt{c}} + \frac{\mathrm{i}\,\hat{j}\,\sqrt{\hbar\,q\,B}\,\left(a^{\dagger} - a\right)\sqrt{2}}{2\,\sqrt{c}}\right)^2}{2\,m} \tag{3.2.1.1.22}$$

> *simplify*(*expand*((**3.2.1.1.22**)))

$$H = \frac{\hbar\,q\,B\,\left(-1 + 2\,a\,a^{\dagger}\right)}{2\,m\,c} \tag{3.2.1.1.23}$$

> *Library:-SortProducts*((**3.2.1.1.23**), [*Dagger*(a), a], *usecommutator*)

$$H = \frac{\hbar\,q\,B\,\left(1 + 2\,a^{\dagger}\,a\right)}{2\,m\,c} \tag{3.2.1.1.24}$$

This is the Hamiltonian of an harmonic oscillator with frequency $\omega_c = \frac{q\,B}{m}$. The possible values for the energy are known: $E = \hbar\,\omega_c\left(n + \frac{1}{2}\right)$, where n is a positive integer.

>

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

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

> $Setup(spaceindices = lowercaselatin)$

$$[spaceindices = lowercaselatin] \tag{3.2.2.1}$$

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

> $Define(L, r, p)$

$$\text{Defined objects with tensor properties}$$

$$\left\{L, p, r, \gamma_{\mu}, \sigma_{\mu}, \partial_{\mu}, g_{\mu,\nu}, \delta_{\mu,\nu}, \epsilon_{\alpha,\beta,\mu,\nu}\right\} \tag{3.2.2.2}$$

Now set the related **Commutator** rules for the algebra in tensor notation

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

$$\left[algebrarules = \left\{\left[p_j, p_k\right]_{-} = 0, \left[r_j, p_k\right]_{-} = \mathrm{i}\,\delta_{j,k}, \left[r_j, r_k\right]_{-} = 0\right\}, quantumoperators = \{L, p, r\}\right] \tag{3.2.2.3}$$

Verify how these algebra rules work:

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

$$\left[r_j, p_k\right]_{-} = \mathrm{i}\,\delta_{j,k} \tag{3.2.2.4}$$

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

$$\left[r_j, r_k\right]_{-} = 0 \tag{3.2.2.5}$$

> $(\%Commutator = Commutator)(p[j], p[k]);$

$$\left[p_j, p_k\right]_{-} = 0 \tag{3.2.2.6}$$

The definition of L_j

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

$$L_j = r_k\,p_m\,\epsilon_j^{\;k,m} \tag{3.2.2.7}$$

The rule to be verified

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

$$[L_j, L_k]_- = \mathrm{i}\,\epsilon_{j,k,m} L^m \quad (3.2.2.8)$$

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

> Library:-SubstituteTensor((3.2.2.7), (3.2.2.8))

$$[r_a p_m \epsilon_j{}^{a,m}, r_b p_c \epsilon_k{}^{b,c}]_- = \mathrm{i}\,\epsilon_{j,k,m} r_a p_b \epsilon^{m,a,b} \quad (3.2.2.9)$$

> Simplify((3.2.2.9))

$$-\mathrm{i}\, r_k p_j + \mathrm{i}\, r_j p_k = -\mathrm{i}\, r_k p_j + \mathrm{i}\, r_j p_k \quad (3.2.2.10)$$

Or one step at a time,

> expand((3.2.2.9))

$$\epsilon_j{}^{a,m} \epsilon_k{}^{b,c} r_a p_m r_b p_c - \epsilon_j{}^{a,m} \epsilon_k{}^{b,c} r_b p_c r_a p_m = \mathrm{i}\,\epsilon_{j,k,m} \epsilon^{a,b,m} r_a p_b \quad (3.2.2.11)$$

> Simplify((3.2.2.11))

$$-\mathrm{i}\, r_k p_j + \mathrm{i}\, r_j p_k = -\mathrm{i}\, r_k p_j + \mathrm{i}\, r_j p_k \quad (3.2.2.12)$$

>

Unitary Operators in Quantum Mechanics

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

A linear operator U is unitary if $U^{-1} = U^{\dagger}$, in which case, $U \cdot U^{\dagger} = U^{\dagger} \cdot U = 1$. Unitary operators are used to change the basis inside an Hilbert space, which physically means changing the point of view of the considered problem, but not the underlying physics. Examples: translations, rotations and the parity operator.

1) 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 $e^{\mathrm{i}\lambda H}$ is unitary provided H is Hermitian ($H = H^{\dagger}$) and λ is any real parameter.

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

> Setup(mathematicalnotation = true, unitaryoperators = {U}, quantumoperators

$= \{V\}, hermitianoperators = \{H\}, realobjects = \{\lambda\})$

$$[hermitianoperators = \{H\}, mathematicalnotation = true, quantumoperators = \{H, U, V\}, realobjects = \{\lambda\}, unitaryoperators = \{U\}] \quad (3.2.3.1.1)$$

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

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

$$U|U_\varepsilon\rangle = \varepsilon |U_\varepsilon\rangle \quad (3.2.3.1.2)$$

> $Dagger(\textbf{(3.2.3.1.2)})$

$$\langle U_\varepsilon | U^\dagger = \bar{\varepsilon} \langle U_\varepsilon | \quad (3.2.3.1.3)$$

Multiplying eq. **(3.2.3.1.3)** and **(3.2.3.1.2)** sides by sides

> **(3.2.3.1.3)** . **(3.2.3.1.2)**

$$1 = |\varepsilon|^2 \quad (3.2.3.1.4)$$

Step by step using `*` instead of `.`

> **(3.2.3.1.3)**·**(3.2.3.1.2)**

$$\langle U_\varepsilon | U^\dagger U | U_\varepsilon \rangle = \bar{\varepsilon}\, \varepsilon \langle U_\varepsilon || U_\varepsilon \rangle \quad (3.2.3.1.5)$$

> $Simplify(\textbf{(3.2.3.1.5)})$

$$\langle U_\varepsilon || U_\varepsilon \rangle = \bar{\varepsilon}\, \varepsilon \langle U_\varepsilon || U_\varepsilon \rangle \quad (3.2.3.1.6)$$

> $subs(`*` = `.`, \textbf{(3.2.3.1.6)})$

$$\langle U_\varepsilon | \bullet | U_\varepsilon \rangle = \bar{\varepsilon}\, \varepsilon (\langle U_\varepsilon | \bullet | U_\varepsilon \rangle) \quad (3.2.3.1.7)$$

> $convert(\textbf{(3.2.3.1.7)}, \mathrm{abs})$

$$1 = |\varepsilon|^2 \quad (3.2.3.1.8)$$

Show that $e^{i \lambda H}$ is unitary

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

$$V = e^{i \lambda H} \quad (3.2.3.1.9)$$

> $Dagger(\textbf{(3.2.3.1.9)})$

$$V^\dagger = e^{-i \lambda H} \quad (3.2.3.1.10)$$

> **(3.2.3.1.9)** . **(3.2.3.1.10)**

(3.2.3.1.11)

$$V V^{\dagger} = 1 \quad \textbf{(3.2.3.1.11)}$$

> **(3.2.3.1.10)** . **(3.2.3.1.9)**

$$V^{\dagger} V = 1 \quad \textbf{(3.2.3.1.12)}$$

Therefore, V is unitary

>

2) 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 Hilbert space. Then one can always build an unitary operator U that maps one basis to the other, i.e.:

$$| b_n \rangle = U | a_n \rangle$$

The demonstration is performed for discrete basis sets, but it can be done the same way in the continuous case.

2.1) Verify that $U = \sum_{k=0}^{\infty} | b_k \rangle \langle a_k |$ implies on $| b_n \rangle = U | a_n \rangle$

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

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

$$\left[bracketrules = \left\{\langle a_m | a_n \rangle = \delta_{m,n}, \langle b_m | b_n \rangle = \delta_{m,n}\right\}, quantumdiscretebasis = \{a, b\}, quantumoperators = \{U\}\right] \quad \textbf{(3.2.3.2.1.1)}$$

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

$$U = \sum_{k=0}^{\infty} | b_k \rangle \langle a_k | \quad \textbf{(3.2.3.2.1.2)}$$

> **(3.2.3.2.1.2)** . *Ket*(*a*, *m*)

$$U \bullet | a_m \rangle = | b_m \rangle \quad \textbf{(3.2.3.2.1.3)}$$

Step by step

> **(3.2.3.2.1.2)** $\cdot$ $Ket(a, m)$

$$U\,|a_m\rangle = \left(\sum_{k=0}^{\infty} |b_k\rangle\,\langle a_k|\right)|a_m\rangle \qquad \textbf{(3.2.3.2.1.4)}$$

> $combine$(**(3.2.3.2.1.4)**)

$$U\,|a_m\rangle = \sum_{k=0}^{\infty} |b_k\rangle\,\langle a_k|\,|a_m\rangle \qquad \textbf{(3.2.3.2.1.5)}$$

> $subs$(`*` = `.` , %)

$$U \cdot |a_m\rangle = \sum_{k=0}^{\infty} |b_k\rangle \cdot \langle a_k| \cdot |a_m\rangle \qquad \textbf{(3.2.3.2.1.6)}$$

> **(3.2.3.2.1.6)**

$$U \cdot |a_m\rangle = \sum_{k=0}^{\infty} \delta_{k,\,m}\,|b_k\rangle \qquad \textbf{(3.2.3.2.1.7)}$$

> $Simplify$(**(3.2.3.2.1.7)**)

$$U \cdot |a_m\rangle = |b_m\rangle \qquad \textbf{(3.2.3.2.1.8)}$$

>

2.2) Show, *in steps*, that $U = \sum_{k=0}^{\infty} |b_k\rangle\,\langle a_k|$ is unitary

Recalling the expansion of the test operator U

> **(3.2.3.2.1.2)**

$$U = \sum_{k=0}^{\infty} |b_k\rangle\,\langle a_k| \qquad \textbf{(3.2.3.2.2.1)}$$

We have, in steps,

> **(3.2.3.2.1.2)** $\cdot$ $subs(k = n, Dagger($**(3.2.3.2.1.2)**$))$

$$U\,U^{\dagger} = \left(\sum_{k=0}^{\infty} |b_k\rangle\,\langle a_k|\right)\left(\sum_{n=0}^{\infty} |a_n\rangle\,\langle b_n|\right) \qquad \textbf{(3.2.3.2.2.2)}$$

> $combine$(**(3.2.3.2.2.2)**)

(3.2.3.2.2.3)

$$U\,U^{\dagger} = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} |b_k\rangle\langle a_k||a_n\rangle\langle b_n| \tag{3.2.3.2.2.3}$$

> $subs(`*` = `.`, \mathbf{(3.2.3.2.2.3)})$

$$U\cdot U^{\dagger} = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} |b_k\rangle\cdot\langle a_k|\cdot|a_n\rangle\cdot\langle b_n| \tag{3.2.3.2.2.4}$$

> **(3.2.3.2.2.4)**

$$U\,U^{\dagger} = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} \delta_{k,n}|b_k\rangle\langle b_n| \tag{3.2.3.2.2.5}$$

> $Simplify(\mathbf{(3.2.3.2.2.5)})$

$$U\,U^{\dagger} = \sum_{k=0}^{\infty} |b_k\rangle\langle b_k| \tag{3.2.3.2.2.6}$$

In the same way one arrives to $U^{\dagger}\,U = \sum_{k1=0}^{\infty}|a_{k1}\rangle\langle a_{k1}|$. The same results can be obtained in one go by using the dot product instead of the star product, as in

> **(3.2.3.2.1.2)** . **(3.2.3.2.1.2)***

$$U\,U^{\dagger} = \sum_{k1=0}^{\infty} |b_{k1}\rangle\langle b_{k1}| \tag{3.2.3.2.2.7}$$

> **(3.2.3.2.1.2)*** . **(3.2.3.2.1.2)**

$$U^{\dagger}\,U = \sum_{k1=0}^{\infty} |a_{k1}\rangle\langle a_{k1}| \tag{3.2.3.2.2.8}$$

and since $|a_n\rangle$ and $|b_n\rangle$ form two complete basis, their Kets satisfy the following closure relations:

> $Projector(Ket(a, k), dimension = 0..\infty) = 1,\ Projector(Ket(b, k), dimension = 0..\infty) = 1$

$$\sum_{k=0}^{\infty}|a_k\rangle\langle a_k| = 1, \sum_{k=0}^{\infty}|b_k\rangle\langle b_k| = 1 \tag{3.2.3.2.2.9}$$

Hence U is unitary.

>

2.3) Show that the matrix elements of U in the $|a_n\rangle$ and $|b_n\rangle$ basis are equal

> **(3.2.3.2.1.2)**

$$U = \sum_{k=0}^{\infty} | b_k \rangle \langle a_k | \tag{3.2.3.2.3.1}$$

> $Bra(a, n)$. **(3.2.3.2.1.2)** . $Ket(a, m)$

$$\langle a_n | U | a_m \rangle = \langle a_n | b_m \rangle \tag{3.2.3.2.3.2}$$

Likewise

> $Bra(b, n)$. **(3.2.3.2.1.2)** . $Ket(b, m)$

$$\langle b_n | U | b_m \rangle = \langle a_n | b_m \rangle \tag{3.2.3.2.3.3}$$

>

2.4) Show that A and $\mathcal{A} = U\,A\,U^{\dagger}$ have the same spectrum

If $\mathcal{A} = U\,A\,U^{\dagger}$, then by definition the eigenkets of $\mathcal{A}$ are $| \mathcal{A}_{\alpha} \rangle = U | A_{\alpha} \rangle$ and we need to prove that $\mathcal{A} | \mathcal{A}_{\alpha} \rangle = \alpha | \mathcal{A}_{\alpha} \rangle$

> $Setup(redo, quantumoperators = \{A, \mathcal{A}\}, unitaryoperators = \{U\})$

$$[quantumoperators = \{\mathcal{A}, A, U\}, unitaryoperators = \{U\}] \tag{3.2.3.2.4.1}$$

> $U . Ket(A, \alpha) = Ket(\mathcal{A}, \alpha)$

$$U \bullet | A_{\alpha} \rangle = | \mathcal{A}_{\alpha} \rangle \tag{3.2.3.2.4.2}$$

> $U\,A\,Dagger(U) = \mathcal{A}$

$$U\,A\,U^{\dagger} = \mathcal{A} \tag{3.2.3.2.4.3}$$

Multiply these two equations and use * instead of . , in order to have the product represented but not computed

> **(3.2.3.2.4.3)** · **(3.2.3.2.4.2)**

$$U\,A\,U^{\dagger} \left(U \bullet | A_{\alpha} \rangle\right) = \mathcal{A} | \mathcal{A}_{\alpha} \rangle \tag{3.2.3.2.4.4}$$

The left-hand side can be rewritten performing the product

> $lhs($**(3.2.3.2.4.4)**$) = eval(lhs($**(3.2.3.2.4.4)**$),$ \`*\` = \`.\`$)$

$$U\,A\,U^{\dagger} \left(U \bullet | A_{\alpha} \rangle\right) = \alpha \left(U \bullet | A_{\alpha} \rangle\right) \tag{3.2.3.2.4.5}$$

> $subs((3.2.3.2.4.5), (3.2.3.2.4.4))$

$$\alpha \left(U \cdot \left| A_{\alpha} \right\rangle\right) = \mathcal{A} \left| \mathcal{A}_{\alpha} \right\rangle \quad (3.2.3.2.4.6)$$

> $subs((3.2.3.2.4.2), (3.2.3.2.4.6))$

$$\alpha \left| \mathcal{A}_{\alpha} \right\rangle = \mathcal{A} \left| \mathcal{A}_{\alpha} \right\rangle \quad (3.2.3.2.4.7)$$

In conclusion, after an unitary transform, an eigenvector of the initial operator is an eigenvector of the new operator with the same eigenvalue.

>

3) Schrödinger equation and unitary transform

Consider a ket $\left| \psi_t \right\rangle$ that solves the time-dependant Schrödinger equation:

$$\mathrm{i} \cdot \hbar \frac{\partial}{\partial t} \left| \psi_t \right\rangle = H(t) \left| \psi_t \right\rangle$$

and consider

$$\left| \phi_t \right\rangle = U(t) \left| \psi_t \right\rangle,$$

where $U(t)$ is a unitary operator.

Does $\left| \phi_t \right\rangle$ evolves according a Schrödinger equation

$$\mathrm{i} \cdot \hbar \frac{\partial}{\partial t} \left| \phi_t \right\rangle = \mathcal{H}(t) \left| \phi_t \right\rangle$$

and if yes, which is the expression of $\mathcal{H}(t)$?

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

> $Setup(mathematicalnotation = true, quantumoperators = \{\mathcal{H}\}, hermitianoperators = \{H\}, unitaryoperators = \{U\}, realobjects = \{t, \hbar\})$

$$[hermitianoperators = \{H\}, mathematicalnotation = true, quantumoperators = \{\mathcal{H}, H, U\}, realobjects = \{\hbar, t\}, unitaryoperators = \{U\}] \quad (3.2.3.3.1)$$

> $PDEtools\text{:-}declare((U, H, \mathcal{H})(t))$

$U(t)$ *will now be displayed as* U

$$H(t) \text{ will now be displayed as } H$$
$$\mathcal{H}(t) \text{ will now be displayed as } \mathcal{H} \quad \textbf{(3.2.3.3.2)}$$

> $Ket(\phi, t) = U(t) \cdot Ket(\psi, t)$

$$\left|\phi_t\right\rangle = U\left|\psi_t\right\rangle \quad \textbf{(3.2.3.3.3)}$$

Since U is unitary, this equation also implies on

> $simplify\left(U(t)^* \cdot (rhs = lhs)(\textbf{(3.2.3.3.3)})\right)$

$$\left|\psi_t\right\rangle = U^\dagger\left|\phi_t\right\rangle \quad \textbf{(3.2.3.3.4)}$$

Compute now the evolution of $\left|\phi_t\right\rangle$

> $\mathrm{i} \cdot \hbar \cdot diff(\textbf{(3.2.3.3.3)}, t)$

$$\mathrm{i}\,\hbar\left|\phi_t\right\rangle_t = \mathrm{i}\,\hbar\left(U_t\left|\psi_t\right\rangle + U\left|\psi_t\right\rangle_t\right) \quad \textbf{(3.2.3.3.5)}$$

Simlpify this equation taking into account Schrödinger's equation for ψ :

> $\mathrm{i} \cdot \hbar\, \frac{\partial}{\partial t} Ket(\psi, t) = H(t)\, Ket(\psi, t)$

$$\mathrm{i}\,\hbar\left|\psi_t\right\rangle_t = H\left|\psi_t\right\rangle \quad \textbf{(3.2.3.3.6)}$$

> $simplify\left(\textbf{(3.2.3.3.5)}, \{\textbf{(3.2.3.3.6)}\}, \left\{\frac{\partial}{\partial t} Ket(\psi, t)\right\}\right)$

$$\mathrm{i}\,\hbar\left|\phi_t\right\rangle_t = \mathrm{i}\,\hbar\left(-\frac{\mathrm{i}\, U\, H\left|\psi_t\right\rangle}{\hbar} + U_t\left|\psi_t\right\rangle\right) \quad \textbf{(3.2.3.3.7)}$$

Inserting here $\left|\psi_t\right\rangle = U^\dagger\left|\phi_t\right\rangle$

> $subs(\textbf{(3.2.3.3.4)}, \textbf{(3.2.3.3.7)})$

$$\mathrm{i}\,\hbar\left|\phi_t\right\rangle_t = \mathrm{i}\,\hbar\left(-\frac{\mathrm{i}\, U\, H\left(U^\dagger\left|\phi_t\right\rangle\right)}{\hbar} + U_t\left(U^\dagger\left|\phi_t\right\rangle\right)\right) \quad \textbf{(3.2.3.3.8)}$$

Therefore, $\left|\phi_t\right\rangle$ evolves according a Schrödinger equation where the $\mathcal{H}$amiltonian is given by

> $\mathcal{H}(t) = Coefficients\left(\mathrm{rhs}(\textbf{(3.2.3.3.8)}), Ket(\phi, t)\right)$

$$\mathcal{H} = \mathrm{i}\,\hbar\, U_t\, U^\dagger + U\, H\, U^\dagger \quad \textbf{(3.2.3.3.9)}$$

Since $\mathcal{H}$ is a Hamiltonian, it must be Hermitian

> $simplify(Dagger(\textbf{(3.2.3.3.9)}) - \textbf{(3.2.3.3.9)}, size)$

$$\mathcal{H}^\dagger - \mathcal{H} = -\mathrm{i}\,\hbar\left(U_t\, U^\dagger + U\, {U^\dagger}_t\right) \quad \textbf{(3.2.3.3.10)}$$

Recalling that $U(t)$ satisfies

> $U(t) \cdot U(t)^* = U(t) \bullet U(t)^*$

$$U\, U^{\dagger} = 1 \qquad \textbf{(3.2.3.3.11)}$$

> $diff(\textbf{(3.2.3.3.11)}, t)$

$$U_t\, U^{\dagger} + U\, {U^{\dagger}}_t = 0 \qquad \textbf{(3.2.3.3.12)}$$

> $subs(\textbf{(3.2.3.3.12)}, \textbf{(3.2.3.3.10)})$

$$\mathcal{H}^{\dagger} - \mathcal{H} = 0 \qquad \textbf{(3.2.3.3.13)}$$

>

4) Translation operators

In this section, we build two unitary operators: $U(t) = \mathrm{e}^{\frac{-\mathrm{i}\, p(t)\, X}{\hbar}}$ and $T(t) = \mathrm{e}^{\frac{-\mathrm{i}\, x(t)\, P}{\hbar}}$, where X is the position operator along the x axis, P the momentum operator along the same axis; $p(t)$ and $x(t)$ are arbitrary time dependent real parameters. Since both X and P are Hermitian, according to section 1, $U(t)$ and $T(t)$ are unitary. Additionally, there is an important property that should be taken into account, X and P do not commute:

$$[X, P]_{-} = \mathrm{i}\, \hbar$$

$$[A, f(B)]_{-} = [A, B]_{-} \frac{\mathrm{d}}{\mathrm{d}B} f(B)$$

4.1) $U(t) = \mathrm{e}^{\frac{-\mathrm{i}\, p(t)\, X}{\hbar}}$ induces a translation of p

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

> $PDEtools\text{:-}declare((p, x, U, T)(t))$

$p(t)$ *will now be displayed as* p
$x(t)$ *will now be displayed as* x
$U(t)$ *will now be displayed as* U
$T(t)$ *will now be displayed as* T **(3.2.3.4.1.1)**

> $Setup\big(mathematicalnotation = true, hermitianoperators = \{P, X, H\}, quantumoperators = \{U, T\}, realobjects = \{t, \hbar, a, p(t), x(t), \theta\}\big)$

$[hermitianoperators = \{H, P, X\}, mathematicalnotation = true,$ **(3.2.3.4.1.2)**

$$quantumoperators = \{H, P, T, U, X\}, realobjects = \{\hbar, a, t, \theta, p, x\}]$$

> $Setup(algebrarules = \{\%Commutator(X, P) = \mathrm{i}\cdot\hbar\})$

$$[algebrarules = \{[X, P]_- = \mathrm{i}\,\hbar\}] \quad \textbf{(3.2.3.4.1.3)}$$

> $U(t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\,X\,p(t)\right)$

$$U = \mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}} \quad \textbf{(3.2.3.4.1.4)}$$

First, since $U(t)$ commutes with X, U has no effect on X

> $\textbf{(3.2.3.4.1.4)}\cdot X\cdot\textbf{(3.2.3.4.1.4)}^*$

$$U\,X\,U^\dagger = \mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}}\,X\,\mathrm{e}^{\frac{\mathrm{i}\,p\,X}{\hbar}} \quad \textbf{(3.2.3.4.1.5)}$$

> $simplify(\textbf{(3.2.3.4.1.5)})$

$$U\,X\,U^\dagger = X \quad \textbf{(3.2.3.4.1.6)}$$

Now, let's evaluate how P is transformed by U

> $\textbf{(3.2.3.4.1.4)}\cdot P\cdot\textbf{(3.2.3.4.1.4)}^*$

$$U\,P\,U^\dagger = \mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}}\,P\,\mathrm{e}^{\frac{\mathrm{i}\,p\,X}{\hbar}} \quad \textbf{(3.2.3.4.1.7)}$$

For that purpose, one needs to know the commutator between P and U, in turn a consequence of $= i\,\hbar$

> $(\%Commutator = Commutator)\left(P, \exp\left(-\frac{\mathrm{i}}{\hbar}\,X\,p(t)\right)\right)$

$$\left[P, \mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}}\right]_- = -p\,\mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}} \quad \textbf{(3.2.3.4.1.8)}$$

Let's add this commutator explicitly

> $Setup(\textbf{(3.2.3.4.1.8)}):$

Now the operation can be simplified

> **(3.2.3.4.1.7)**

$$U\,P\,U^\dagger = \mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}}\,P\,\mathrm{e}^{\frac{\mathrm{i}\,p\,X}{\hbar}} \quad \textbf{(3.2.3.4.1.9)}$$

> $SortProducts\left(\textbf{(3.2.3.4.1.9)}, \left[P, \exp\left(\frac{-\mathrm{i}\,X\,p(t)}{\hbar}\right)\right], usecommutator\right)$

$$U\,P\,U^\dagger = \left(P\,\mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}} + p\,\mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}}\right)\mathrm{e}^{\frac{\mathrm{i}\,p\,X}{\hbar}} \quad \textbf{(3.2.3.4.1.10)}$$

> $simplify(\textbf{(3.2.3.4.1.10)})$

(3.2.3.4.1.11)

$$U\,P\,U^{\dagger} = P + p \qquad \textbf{(3.2.3.4.1.11)}$$

Therefore, P has been translated by an amount $p(t)$.

>

This result can be generalized to arbitrary powers of P.

> **(3.2.3.4.1.4)**$\cdot P^2 \cdot$**(3.2.3.4.1.4)***

$$U\,P^2\,U^{\dagger} = \mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}}\,P^2\,\mathrm{e}^{\frac{\mathrm{i}\,p\,X}{\hbar}} \qquad \textbf{(3.2.3.4.1.1.1)}$$

> $SortProducts\left(\textbf{(3.2.3.4.1.1.1)}, \left[P, \exp\left(\frac{-\mathrm{i}\,X\,p(t)}{\hbar}\right)\right], usecommutator\right)$

$$U\,P^2\,U^{\dagger} = \left(P\,\mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}} + p\,\mathrm{e}^{\frac{-\mathrm{i}\,p\,X}{\hbar}}\right)P\,\mathrm{e}^{\frac{\mathrm{i}\,p\,X}{\hbar}} \qquad \textbf{(3.2.3.4.1.1.2)}$$

> $Simplify($**(3.2.3.4.1.1.2)**$)$

$$U\,P^2\,U^{\dagger} = P^2 + 2\,p\,P + p^2 \qquad \textbf{(3.2.3.4.1.1.3)}$$

> $(P + p(t))^2$

$$(P + p)^2 \qquad \textbf{(3.2.3.4.1.1.4)}$$

> $expand($**(3.2.3.4.1.1.4)**$) =$ **(3.2.3.4.1.1.4)**

$$P^2 + 2\,p\,P + p^2 = (P + p)^2 \qquad \textbf{(3.2.3.4.1.1.5)}$$

> $lhs($**(3.2.3.4.1.1.3)**$) = simplify(rhs($**(3.2.3.4.1.1.3)**$), \{$**(3.2.3.4.1.1.5)**$\})$

$$U\,P^2\,U^{\dagger} = (P + p)^2 \qquad \textbf{(3.2.3.4.1.1.6)}$$

It's possible to demonstrate the general relation: $U \cdot P^n \cdot U^{\dagger} = (P + p)^n$, where n is a positive integer. The result has been demonstrated above for $n = 1$ and $n = 2$. Assuming that the equality is valid up-to n, let's demonstrate it for $n + 1$. Indeed, since $U^{\dagger}\,U = 1$:

$$U\,P^{n+1}\,U^{\dagger} = U\,P^n\,P\,U^{\dagger} = U\,P^n\,U^{\dagger}\,U\,P\,U^{\dagger} = (P + p)^n\,(P + p) = (P + p)^{n+1}$$

So, in a general manner, given f, a commutative mapping that can be decomposed into a formal power series in all the complex plan, one have:

$$\mathrm{e}^{\frac{-\mathrm{i}\,p(t)\,X}{\hbar}}\,f(P)\,\mathrm{e}^{\frac{\mathrm{i}\,p(t)\,X}{\hbar}} = f(P + p(t))$$

From where $e^{\frac{-i p(t) X}{\hbar}} f(P)\, e^{\frac{i p(t) X}{\hbar}}$ is a translated copy of $f(P)$ by an amount $-p(t)$.

4.2) $T(t) = e^{\frac{-i x(t) P}{\hbar}}$ induces a translation of x

> $T(t) = \exp\left(-\frac{i}{\hbar} P\, x(t)\right)$

$$T = e^{\frac{-i x P}{\hbar}} \quad \textbf{(3.2.3.4.2.1)}$$

Like in the previous section, $T(t)$ commutes with P; T leaves then P unchanged

> $\mathit{Simplify}\left(\textbf{(3.2.3.4.2.1)} \cdot P \cdot \textbf{(3.2.3.4.2.1)}^{*}\right)$

$$T\, P\, T^{\dagger} = e^{\frac{-i x P}{\hbar}}\, P\, e^{\frac{i x P}{\hbar}} \quad \textbf{(3.2.3.4.2.2)}$$

> $(\%\mathit{Commutator} = \mathit{Commutator})\left(X, \exp\left(-\frac{i}{\hbar} P\, x(t)\right)\right)$

$$\left[X, e^{\frac{-i x P}{\hbar}}\right]_{-} = x\, e^{\frac{-i x P}{\hbar}} \quad \textbf{(3.2.3.4.2.3)}$$

> $\mathit{Setup}(\textbf{(3.2.3.4.2.3)}) :$

Evaluating now

> $\textbf{(3.2.3.4.2.1)} \cdot X \cdot \textbf{(3.2.3.4.2.1)}^{*}$

$$T\, X\, T^{\dagger} = e^{\frac{-i x P}{\hbar}}\, X\, e^{\frac{i x P}{\hbar}} \quad \textbf{(3.2.3.4.2.4)}$$

> $\mathit{SortProducts}\left(\textbf{(3.2.3.4.2.4)}, \left[X, \exp\left(\frac{-i\, P\, x(t)}{\hbar}\right)\right], \mathit{usecommutator}\right)$

$$T\, X\, T^{\dagger} = \left(X\, e^{\frac{-i x P}{\hbar}} - x\, e^{\frac{-i x P}{\hbar}}\right) e^{\frac{i x P}{\hbar}} \quad \textbf{(3.2.3.4.2.5)}$$

> $\mathit{expand}(\textbf{(3.2.3.4.2.5)})$

$$T\, X\, T^{\dagger} = X - x \quad \textbf{(3.2.3.4.2.6)}$$

>

Classical Field Theory

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.

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

> $interface(imaginaryunit = i) :$

> $macro(\mathrm{Psi} = \mathrm{psi}(x, y, z, t)) :$

> $PDEtools\text{:-}declare((\psi, V)(x, y, z, t))$

$\psi(x, y, z, t)$ *will now be displayed as* ψ

$V(x, y, z, t)$ *will now be displayed as* V **(3.3.1.1.1)**

The energy density E for a quantum system of identical boson particles is (see [3])

> $E := \frac{\hbar^2}{2\,m} Norm(\%Gradient(\mathrm{Psi}))^2 + V(x, y, z, t)\,\mathrm{abs}(\mathrm{Psi})^2 + \frac{G}{2}\,\mathrm{abs}(\mathrm{Psi})^4;$

$$E := \frac{\hbar^2\,\|\nabla\psi\|^2}{2\,m} + V\,|\psi|^2 + \frac{G\,|\psi|^4}{2} \quad \textbf{(3.3.1.1.2)}$$

$\psi(x, y, z, t)$ 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

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

$$L := \frac{\mathrm{i}\,\hbar\left(\overline{\psi}\,\psi_t - \psi\,\overline{\psi}_t\right)}{2} - \frac{\hbar^2\,\|\nabla\psi\|^2}{2\,m} - V\,|\psi|^2 - \frac{G\,|\psi|^4}{2} \quad (3.3.1.1.3)$$

Construct the action and equate to zero the functional derivative

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

$$\left(\frac{\delta}{\delta\,\psi}\right)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{\mathrm{i}\,\hbar\left(\overline{\psi}\,\psi_t - \psi\,\overline{\psi}_t\right)}{2} - \frac{\hbar^2\,\|\nabla\psi\|^2}{2\,m} - V\,|\psi|^2 - \frac{G\,|\psi|^4}{2}\right)\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}t = 0 \quad (3.3.1.1.4)$$

> **(3.3.1.1.4)**

$$\frac{\hbar^2\,\overline{\psi}_{x,x} + \overline{\psi}_{y,y}\,\hbar^2 + \hbar^2\,\overline{\psi}_{z,z} - 2\,m\left(G\,\overline{\psi}^2\,\psi + \mathrm{i}\,\overline{\psi}_t\,\hbar + \overline{\psi}\,V\right)}{2\,m} = 0 \quad (3.3.1.1.5)$$

Make the Laplacian explicit

> (Laplacian = %Laplacian)(Psi)

$$\psi_{x,x} + \psi_{y,y} + \psi_{z,z} = \nabla^2\psi \quad (3.3.1.1.6)$$

> simplify(conjugate(**(3.3.1.1.5)**), {**(3.3.1.1.6)**})

$$\frac{\hbar^2\,\nabla^2\psi}{2\,m} + \frac{-2\,G\,\psi^2\,\overline{\psi}\,m + 2\,\mathrm{i}\,\hbar\,\psi_t\,m - 2\,\psi\,V\,m}{2\,m} = 0 \quad (3.3.1.1.7)$$

The standard form of the Gross–Pitaevskii equation:

> i ħ isolate(**(3.3.1.1.7)**, diff(Psi, t))

$$\mathrm{i}\,\psi_t\,\hbar = \frac{-\frac{\hbar^2\,\nabla^2\psi}{2} + G\,\psi^2\,\overline{\psi}\,m + \psi\,V\,m}{m} \quad (3.3.1.1.8)$$

> collect(convert(expand(**(3.3.1.1.8)**), abs), psi)

$$\mathrm{i}\,\psi_t\,\hbar = \left(G\,|\psi|^2 + V\right)\psi - \frac{\hbar^2\,\nabla^2\psi}{2\,m} \quad (3.3.1.1.9)$$

>

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

The Lagrangian of the $\lambda\,\Phi^4$ model, the corresponding Action, and the field equations:

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

> *Coordinates*(*X*)

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

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

$$\{X\} \tag{3.3.2.1}$$

> *PDEtools*:-*declare*($\Phi(X)$)

$\Phi(x1, x2, x3, x4)$ *will now be displayed as* Φ **(3.3.2.2)**

> $L := \frac{1}{2}\, d_{\_\mu}(\Phi(X))\, d_{\_\mu}(\Phi(X)) - \frac{m^2}{2}\,\Phi(X)^2 + \left(\frac{\lambda}{4}\,\Phi(X)^4\right)$

$$L := \frac{\left(\partial_{\mu}(\Phi)\right)\left(\partial^{\mu}(\Phi)\right)}{2} - \frac{m^2\,\Phi^2}{2} + \frac{\lambda\,\Phi^4}{4} \tag{3.3.2.3}$$

> $S := Intc(L, X)$

$$S := \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\frac{\left(\partial_{\mu}(\Phi)\right)\left(\partial^{\mu}(\Phi)\right)}{2} - \frac{m^2\,\Phi^2}{2} + \frac{\lambda\,\Phi^4}{4}\right) dx1\, dx2\, dx3\, dx4 \tag{3.3.2.4}$$

> '*Fundiff*'(S, Φ)

$$\left(\frac{\delta}{\delta\,\Phi}\right)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\frac{\left(\partial_{\mu}(\Phi)\right)\left(\partial^{\mu}(\Phi)\right)}{2} - \frac{m^2\,\Phi^2}{2} + \frac{\lambda\,\Phi^4}{4}\right) dx1\, dx2\, dx3\, dx4 \tag{3.3.2.5}$$

> **(3.3.2.5)**

$$-\Box(\Phi) - \Phi\left(-\Phi^2\,\lambda + m^2\right) \tag{3.3.2.6}$$

Maxwell equations departing from the 4-dimensional Action for Electrodynamics

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

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

> $Coordinates(X)$

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

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

$$\{X\} \quad \textbf{(3.3.3.1)}$$

The 4-D electromagnetic potential

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

Defined objects with tensor properties

$$\{A_{\mu}, \gamma_{\mu}, \sigma_{\mu}, X_{\mu}, \partial_{\mu}, g_{\mu,\nu}, \delta_{\mu,\nu}, \epsilon_{\alpha,\beta,\mu,\nu}\} \quad \textbf{(3.3.3.2)}$$

> $PDEtools{:}\text{-}declare(A(X))$

$A(x1, x2, x3, x4)$ *will now be displayed as* A **(3.3.3.3)**

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

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

$$F_{\mu,\nu} := \partial_{\mu}(A_{\nu}) - (\partial_{\nu}(A_{\mu})) \quad \textbf{(3.3.3.4)}$$

Equate to 0 the functional derivative of the corresponding Action

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

$$\left(\frac{\delta}{\delta A_{\rho}}\right) \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\partial_{\mu}(A_{\nu}) - (\partial_{\nu}(A_{\mu}))\right)^2 \,\mathrm{d}x1\,\mathrm{d}x2\,\mathrm{d}x3\,\mathrm{d}x4 = 0 \quad \textbf{(3.3.3.5)}$$

> **(3.3.3.5)**

$$\left(2\left(\partial_{\mu}\left(\partial_{\nu}\left(A^{\nu}\right)\right)\right) - 2\,\Box\left(A_{\mu}\right)\right) g^{\mu,\rho} + \left(-2\,\Box\left(A_{\nu}\right) + 2\left(\partial_{\mu}\left(\partial_{\nu}\left(A^{\mu}\right)\right)\right)\right) g^{\nu,\rho} = 0 \quad \textbf{(3.3.3.6)}$$

Simplify the contracted spacetime indices

> $Simplify(\textbf{(3.3.3.6)})$

$$-4\,\Box\left(A^{\rho}\right) + 4\left(\partial_{\mu}\left(\partial^{\rho}\left(A^{\mu}\right)\right)\right) = 0 \quad \textbf{(3.3.3.7)}$$

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

> $OFF;\ convert(Library{:}\text{-}TensorComponents(\textbf{(3.3.3.7)}), diff)$

$$\left[4\left(\frac{\partial^2}{\partial x2^2} A^1(X)\right) + 4\left(\frac{\partial^2}{\partial x3^2} A^1(X)\right) - 4\left(\frac{\partial^2}{\partial x4^2} A^1(X)\right) - 4\left(\frac{\partial^2}{\partial x1 \partial x2} \right.\right. \quad \textbf{(3.3.3.8)}$$

$$A^2(X)\Big) - 4\left(\frac{\partial^2}{\partial x1 \partial x3} A^3(X)\right) - 4\left(\frac{\partial^2}{\partial x1 \partial x4} A^4(X)\right) = 0, 4\left(\frac{\partial^2}{\partial x1^2} A^2(X)\right) + 4\left(\frac{\partial^2}{\partial x3^2} A^2(X)\right) - 4\left(\frac{\partial^2}{\partial x4^2} A^2(X)\right) - 4\left(\frac{\partial^2}{\partial x1 \partial x2} A^1(X)\right) - 4\left(\frac{\partial^2}{\partial x2 \partial x3} A^3(X)\right) - 4\left(\frac{\partial^2}{\partial x2 \partial x4} A^4(X)\right) = 0, 4\left(\frac{\partial^2}{\partial x1^2} A^3(X)\right) + 4\left(\frac{\partial^2}{\partial x2^2} A^3(X)\right) - 4\left(\frac{\partial^2}{\partial x4^2} A^3(X)\right) - 4\left(\frac{\partial^2}{\partial x1 \partial x3} A^1(X)\right) - 4\left(\frac{\partial^2}{\partial x2 \partial x3} A^2(X)\right) - 4\left(\frac{\partial^2}{\partial x3 \partial x4} A^4(X)\right) = 0, 4\left(\frac{\partial^2}{\partial x1^2} A^4(X)\right) + 4\left(\frac{\partial^2}{\partial x2^2} A^4(X)\right) + 4\left(\frac{\partial^2}{\partial x3^2} A^4(X)\right) + 4\left(\frac{\partial^2}{\partial x1 \partial x4} A^1(X)\right) + 4\left(\frac{\partial^2}{\partial x2 \partial x4} A^2(X)\right) + 4\left(\frac{\partial^2}{\partial x3 \partial x4} A^3(X)\right) = 0\Big]$$

>

General Relativity

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

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

b) Compute the components of

$$W_{\alpha}^{\ \beta} \equiv \text{the traceless part of } Z_{\alpha}^{\ \beta} \text{ of item } \mathbf{a)}$$

c) Compute an exact solution to the nonlinear system of differential equations conformed by the components of $W_{\alpha}^{\ \beta}$ obtained in **b)**

Background: paper from February/2013, "Withholding Potentials, Absence of Ghosts and Relationship between Minimal Dilatonic Gravity and f(R) Theories", by P. Fiziev.

a) The trace of $Z_{\alpha}^{\ \beta} = \Phi R_{\alpha}^{\ \beta} + \mathcal{D}_{\alpha} \mathcal{D}^{\beta} \Phi + T_{\alpha}^{\ \beta}$

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

Set the coordinates

```
> Setup(coordinates = spherical)
```

** Partial match of 'coordinates' against keyword 'coordinatesystems'*

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

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

$$[\mathit{coordinatesystems} = \{X\}] \qquad \textbf{(3.4.1.1)}$$

The square of the line element and the metric

```
> ds2 := exp(nu(r))dt^2 - exp(lambda(r))dr^2 - r^2 dtheta^2 - r^2 sin(theta)^2 dphi^2
```

$$ds2 := \mathrm{e}^{\nu(r)}\, dt^2 - \mathrm{e}^{\lambda(r)}\, dr^2 - r^2\, d\theta^2 - r^2 \sin(\theta)^2\, d\phi^2 \qquad \textbf{(3.4.1.2)}$$

```
> PDEtools:-declare(ds2)
```

$\lambda(r)$ will now be displayed as λ

$\nu(r)$ will now be displayed as ν **(3.4.1.3)**

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

$$g_{\mu, \nu} = \begin{bmatrix} -\mathrm{e}^{\lambda} & 0 & 0 & 0 \\ 0 & -r^2 & 0 & 0 \\ 0 & 0 & -r^2 \sin(\theta)^2 & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\nu} \end{bmatrix} \qquad \textbf{(3.4.1.4)}$$

The indicated stress-energy tensor

```
> T[alpha, beta] = 8·Pi·Matrix(4, ⟨exp(lambda(r)), r^2, r^2 sin(theta)^2,
      epsilon exp(nu(r))⟩, shape = diagonal)
```

$$T_{\alpha,\beta} = \begin{bmatrix} 8\pi e^{\lambda} & 0 & 0 & 0 \\ 0 & 8\pi r^2 & 0 & 0 \\ 0 & 0 & 8\pi r^2 \sin(\theta)^2 & 0 \\ 0 & 0 & 0 & 8\pi \epsilon e^{\nu} \end{bmatrix} \tag{3.4.1.5}$$

> *Define*((**3.4.1.5**))

Defined objects with tensor properties

$$\left\{\mathcal{D}_{\mu}, \gamma_{\mu}, \sigma_{\mu}, R_{\mu,\nu}, R_{\mu,\nu,\alpha,\beta}, T_{\alpha,\beta}, C_{\mu,\nu,\alpha,\beta}, X_{\mu}, \partial_{\mu}, g_{\mu,\nu}, \Gamma_{\mu,\nu,\alpha}, G_{\mu,\nu}, \delta_{\mu,\nu}, \epsilon_{\alpha,\beta,\mu,\nu}\right\} \tag{3.4.1.6}$$

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

> *PDEtools*:-*declare*(Phi(*r*))

$$\Phi(r) \textit{ will now be displayed as } \Phi \tag{3.4.1.7}$$

> *Z*[mu, nu] = Phi(*r*) *Ricci*[mu, nu] +'*D*_[mu](*D*_[nu](Phi(*r*)))'+ *T*[mu, nu]

$$Z_{\mu,\nu} = \Phi R_{\mu,\nu} + \mathcal{D}_{\mu}\left(\mathcal{D}_{\nu}(\Phi)\right) + T_{\mu,\nu} \tag{3.4.1.8}$$

> *Define*((**3.4.1.8**))

Defined objects with tensor properties

$$\left\{\mathcal{D}_{\mu}, \gamma_{\mu}, \sigma_{\mu}, R_{\mu,\nu}, R_{\mu,\nu,\alpha,\beta}, T_{\alpha,\beta}, C_{\mu,\nu,\alpha,\beta}, X_{\mu}, Z_{\mu,\nu}, \partial_{\mu}, g_{\mu,\nu}, \Gamma_{\mu,\nu,\alpha}, G_{\mu,\nu}, \delta_{\mu,\nu}, \epsilon_{\alpha,\beta,\mu,\nu}\right\} \tag{3.4.1.9}$$

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

> *Z*[mu, mu]

$$Z_{\mu}^{\ \mu} \tag{3.4.1.10}$$

> *SumOverRepeatedIndices*((**3.4.1.10**))

$$\frac{\Phi\left(\nu_r^2 r - \nu_r \lambda_r r + 2\nu_{r,r} r - 4\lambda_r\right) e^{-\lambda}}{4r} - e^{-\lambda}\Phi_{r,r} + \frac{\lambda_r e^{-\lambda}\Phi_r}{2} - 24\pi + \frac{\Phi\left(\nu_r e^{-\lambda} r - \lambda_r e^{-\lambda} r + 2e^{-\lambda} - 2\right)}{r^2} - \frac{2e^{-\lambda}\Phi_r}{r} \tag{3.4.1.11}$$

$$+\frac{\Phi e^{-\lambda}\left(\nu_r^{\,2} r-\nu_r\lambda_r r+2\nu_{r,r} r+4\nu_r\right)}{4r}-\frac{\nu_r e^{-\lambda}\Phi_r}{2}+8\pi\epsilon$$

> *show*;

$$\frac{1}{4r}\left(\Phi(r)\left(\left(\frac{d}{dr}\nu(r)\right)^2 r-\left(\frac{d}{dr}\nu(r)\right)\left(\frac{d}{dr}\lambda(r)\right)r+2\left(\frac{d^2}{dr^2}\nu(r)\right)r-4\left(\frac{d}{dr}\lambda(r)\right)\right)e^{-\lambda(r)}\right)-e^{-\lambda(r)}\left(\frac{d^2}{dr^2}\Phi(r)\right)+\frac{\left(\frac{d}{dr}\lambda(r)\right)e^{-\lambda(r)}\left(\frac{d}{dr}\Phi(r)\right)}{2}-24\pi+\frac{\Phi(r)\left(\left(\frac{d}{dr}\nu(r)\right)e^{-\lambda(r)}r-\left(\frac{d}{dr}\lambda(r)\right)e^{-\lambda(r)}r+2e^{-\lambda(r)}-2\right)}{r^2}-\frac{2e^{-\lambda(r)}\left(\frac{d}{dr}\Phi(r)\right)}{r}+\frac{1}{4r}\left(\Phi(r)e^{-\lambda(r)}\left(\left(\frac{d}{dr}\nu(r)\right)^2 r-\left(\frac{d}{dr}\nu(r)\right)\left(\frac{d}{dr}\lambda(r)\right)r+2\left(\frac{d^2}{dr^2}\nu(r)\right)r+4\left(\frac{d}{dr}\nu(r)\right)\right)\right)-\frac{\left(\frac{d}{dr}\nu(r)\right)e^{-\lambda(r)}\left(\frac{d}{dr}\Phi(r)\right)}{2}+8\pi\epsilon \quad \textbf{(3.4.1.12)}$$

>

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

Define a tensor $W_{\mu,\nu}$ with the the traceless part of $Z_{\mu,\nu}$

> $W[\text{mu},\text{nu}]=Z[\text{mu},\text{nu}]-\frac{Z[\text{alpha},\text{alpha}]}{4}g\_[\text{mu},\text{nu}]$

$$W_{\mu,\nu}=Z_{\mu,\nu}-\frac{Z_{\alpha}^{\ \alpha}g_{\mu,\nu}}{4} \quad \textbf{(3.4.2.1)}$$

> *Define*(**(3.4.2.1)**)

Defined objects with tensor properties

$$\{\mathcal{D}_{\mu},\gamma_{\mu},\sigma_{\mu},R_{\mu,\nu},R_{\mu,\nu,\alpha,\beta},T_{\alpha,\beta},W_{\mu,\nu},C_{\mu,\nu,\alpha,\beta},X_{\mu},Z_{\mu,\nu},\partial_{\mu},g_{\mu,\nu},\Gamma_{\mu,\nu,\alpha},G_{\mu,\nu}, \quad \textbf{(3.4.2.2)}$$

$\delta_{\mu,\nu}, \epsilon_{\alpha,\beta,\mu,\nu}\}$

The matrix components for the traceless $W_{\mu}^{\ \nu}$ are then

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

$$W_{\mu}^{\ \nu} = \left[\left[\frac{1}{8 r^2}\left(\left(-6\,\Phi_{r,r}\,r^2 + 2\,\nu_{r,r}\,\Phi\,r^2 + \nu_r^{\,2}\,\Phi\,r^2 - r\left(\lambda_r\,\Phi\,r - \Phi_r\,r + 4\,\Phi\right)\nu_r + \left(3\,r^2\,\Phi_r - 4\,r\,\Phi\right)\lambda_r + 4\,\Phi_r\,r - 4\,\Phi\right)\mathrm{e}^{-\lambda} + 4\,\Phi + (-16\,\epsilon - 16)\,\pi\,r^2\right), 0, 0, 0\right],\right.$$
$$\left[0, \frac{1}{8 r^2}\left(\left(2\,\Phi_{r,r}\,r^2 - 2\,\nu_{r,r}\,\Phi\,r^2 + \left(r^2\,\nu_r - r^2\,\lambda_r - 4\,r\right)\Phi_r - \Phi\left(r^2\,\nu_r^{\,2} - r^2\,\nu_r\,\lambda_r - 4\right)\right)\mathrm{e}^{-\lambda} - 4\,\Phi + (-16\,\epsilon - 16)\,\pi\,r^2\right), 0, 0\right],$$
$$\left[0, 0, \frac{1}{8 r^2}\left(\left(2\,\Phi_{r,r}\,r^2 - 2\,\nu_{r,r}\,\Phi\,r^2 + \left(r^2\,\nu_r - r^2\,\lambda_r - 4\,r\right)\Phi_r - \Phi\left(r^2\,\nu_r^{\,2} - r^2\,\nu_r\,\lambda_r - 4\right)\right)\mathrm{e}^{-\lambda} - 4\,\Phi + (-16\,\epsilon - 16)\,\pi\,r^2\right), 0\right],$$
$$\left.\left[0, 0, 0, \frac{1}{8 r^2}\left(\left(2\,\Phi_{r,r}\,r^2 + 2\,\nu_{r,r}\,\Phi\,r^2 + \nu_r^{\,2}\,\Phi\,r^2 - r\left(\lambda_r\,\Phi\,r + 3\,\Phi_r\,r - 4\,\Phi\right)\nu_r + \left(-r^2\,\Phi_r + 4\,r\,\Phi\right)\lambda_r + 4\,\Phi_r\,r - 4\,\Phi\right)\mathrm{e}^{-\lambda} + 4\,\Phi + (48\,\epsilon + 48)\,\pi\,r^2\right)\right]\right] \quad \textbf{(3.4.2.3)}$$

>

c) An exact solution for the nonlinear system of differential equations conformed by the components of $W_{\alpha}^{\ \beta}$

Create an ODE system with the nonzero components of $W_{\mu}^{\ \nu}$

> $ode_{system} := map(u \rightarrow rhs(u) = 0, rhs(W[\mathrm{mu},\sim\mathrm{nu}, nonzero]))$

$$ode_{system} := \left\{\frac{1}{8 r^2}\left(\left(2\,\Phi_{r,r}\,r^2 - 2\,\nu_{r,r}\,\Phi\,r^2 + \left(r^2\,\nu_r - r^2\,\lambda_r - 4\,r\right)\Phi_r\right.\right.\right. \quad \textbf{(3.4.3.1)}$$

$$- \Phi \left(r^2 \nu_r^2 - r^2 \nu_r \lambda_r - 4\right)\Big) e^{-\lambda} - 4\,\Phi + (-16\,\epsilon - 16)\,\pi\, r^2\Big) = 0,$$

$$\frac{1}{8\,r^2}\Big(\Big(-6\,\Phi_{r,r}\, r^2 + 2\,\nu_{r,r}\,\Phi\, r^2 + \nu_r^2\,\Phi\, r^2 - r\left(\lambda_r\,\Phi\, r - \Phi_r\, r + 4\,\Phi\right)\nu_r$$

$$+ \left(3\,r^2\,\Phi_r - 4\,r\,\Phi\right)\lambda_r + 4\,\Phi_r\, r - 4\,\Phi\Big) e^{-\lambda} + 4\,\Phi + (-16\,\epsilon - 16)\,\pi\, r^2\Big)$$

$$= 0,\ \frac{1}{8\,r^2}\Big(\Big(2\,\Phi_{r,r}\, r^2 + 2\,\nu_{r,r}\,\Phi\, r^2 + \nu_r^2\,\Phi\, r^2 - r\,\big(\lambda_r\,\Phi\, r + 3\,\Phi_r\, r$$

$$- 4\,\Phi\big)\,\nu_r + \left(-r^2\,\Phi_r + 4\,r\,\Phi\right)\lambda_r + 4\,\Phi_r\, r - 4\,\Phi\Big) e^{-\lambda} + 4\,\Phi + (48\,\epsilon$$

$$+ 48)\,\pi\, r^2\Big) = 0\Big\}$$

> *Cases* := *simplify*([*PDEtools*:-*casesplit*(ode_{system})], *size*) :

There are three cases

> *nops*(*Cases*)

$$3 \qquad \textbf{(3.4.3.2)}$$

> *map*(*length*, *Cases*)

$$[5399, 1661, 405] \qquad \textbf{(3.4.3.3)}$$

An exact solution for Cases[3]

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

$$sys_3 := \left[e^{-\lambda} = -\frac{4\,\pi\, r^2\,(\epsilon + 1)}{\Phi},\ \lambda_r = 0,\ \nu_{r,r} = \frac{-r^4\,\pi\,(\epsilon + 1)\,\nu_r^2 + 2\,r^3\,\pi\,(\epsilon + 1)\,\nu_r + \Phi + (4\,\epsilon + 4)\,\pi\, r^2}{2\,r^4\,\pi\,(\epsilon + 1)},\ \Phi_r = \frac{2\,\Phi}{r}\right] \qquad \textbf{(3.4.3.4)}$$

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

$$constraint, subsystem := \left[e^{-\lambda} = -\frac{4\,\pi\, r^2\,(\epsilon + 1)}{\Phi}\right], \left[\lambda_r = 0,\ \nu_{r,r} = \frac{-r^4\,\pi\,(\epsilon + 1)\,\nu_r^2 + 2\,r^3\,\pi\,(\epsilon + 1)\,\nu_r + \Phi + (4\,\epsilon + 4)\,\pi\, r^2}{2\,r^4\,\pi\,(\epsilon + 1)},\ \Phi_r = \frac{2\,\Phi}{r}\right] \qquad \textbf{(3.4.3.5)}$$

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

(3.4.3.6)

$$sol_{subsystem} := \left\{ \Phi = \_C1\, r^2, \nu = -\frac{1}{\sqrt{\pi\,(\epsilon+1)}} \left(\ln\left(\frac{(32\,\epsilon+32)\,\pi + 4\,\_C1}{\pi\,(\epsilon+1)\left(r^{\frac{\sqrt{(8\,\epsilon+8)\,\pi+\_C1}}{\sqrt{\pi\,(\epsilon+1)}}}\,\_C2 - \_C3 \right)^2} \right) \sqrt{\pi\,(\epsilon+1)} + \ln(r)\left(\sqrt{(8\,\epsilon+8)\,\pi+\_C1} - 2\sqrt{\pi\,(\epsilon+1)}\right) \right), \lambda = \_C2 \right\} \quad \textbf{(3.4.3.6)}$$

Specialize one of these constants using the constraint

> *eval*(*constraint*, $sol_{subsystem}$)

$$\left[e^{-\_C2} = -\frac{4\,\pi\,(\epsilon+1)}{\_C1} \right] \quad \textbf{(3.4.3.7)}$$

> *solve*(**(3.4.3.7)**, _C1)

$$\left\{ \_C1 = -\frac{4\,\pi\,(\epsilon+1)}{e^{-\_C2}} \right\} \quad \textbf{(3.4.3.8)}$$

The exact solution

> *solution* := *subs*(**(3.4.3.8)**, $sol_{subsystem}$)

$$solution := \left\{ \Phi = -\frac{4\,\pi\,(\epsilon+1)\,r^2}{e^{-\_C2}}, \nu = -\frac{1}{\sqrt{\pi\,(\epsilon+1)}} \left(\ln\left(\frac{(32\,\epsilon+32)\,\pi - \frac{16\,\pi\,(\epsilon+1)}{e^{-\_C2}}}{\pi\,(\epsilon+1)\left(r^{\frac{\sqrt{(8\,\epsilon+8)\,\pi - \frac{4\,\pi\,(\epsilon+1)}{e^{-\_C2}}}}{\sqrt{\pi\,(\epsilon+1)}}}\,\_C2 - \_C3 \right)^2} \right) \right. \quad \textbf{(3.4.3.9)}$$

$$\sqrt{\pi\,(\epsilon+1)} + \ln(r)\left(\sqrt{(8\,\epsilon+8)\,\pi - \frac{4\,\pi\,(\epsilon+1)}{e^{-\_C2}}} - 2\sqrt{\pi\,(\epsilon+1)}\right)\Bigg), \lambda$$

$$= \_C2 \Bigg\}$$

Verifying this result

> $odetest\left(solution, ode_{system}\right)$

$$\{0\} \qquad \textbf{(3.4.3.10)}$$

>

The Physics Project

"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 searcheable 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.