

Title: Computer Algebra for Theoretical Physics

Date: Oct 07, 2014 10:00 AM

URL: <http://pirsa.org/14100068>

Abstract: 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. Feel free to join!

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We can share results in a reproducible way

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Vector and tensor notation in special and general relativity

Formalism	Formulation	Homogeneous equations	Non-homogeneous equations
Vector calculus	Fields 3D Euclidean space + time	$\nabla \cdot \mathbf{B} = 0$ $\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0$	$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$ $\nabla \times \mathbf{B} - \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J}$
	Potentials (any gauge) 3D Euclidean space + time	$\mathbf{B} = \nabla \times \mathbf{A}$ $\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}$	$\nabla^2 \varphi + \frac{\partial}{\partial t} (\nabla \cdot \mathbf{A}) = -\frac{\rho}{\epsilon_0}$ $\square \mathbf{A} + \nabla \left(\nabla \cdot \mathbf{A} + \frac{1}{c^2} \frac{\partial \varphi}{\partial t} \right) = \mu_0 \mathbf{J}$
	Potentials (Lorenz gauge) 3D Euclidean space + time	$\mathbf{B} = \nabla \times \mathbf{A}$ $\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}$ $\nabla \cdot \mathbf{A} + \frac{1}{c^2} \frac{\partial \varphi}{\partial t} = 0$	$\square \varphi = \frac{\rho}{\epsilon_0}$ $\square \mathbf{A} = \mu_0 \mathbf{J}$
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	$F_{\alpha\beta} = \partial_{[\alpha} A_{\beta]}$ $\partial_\alpha A^\alpha = 0$	$\square A^\alpha = -\mu_0 J^\alpha$
	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	$F_{\alpha\beta} = \partial_{[\alpha} A_{\beta]} = \nabla_{[\alpha} A_{\beta]}$	$\nabla_\alpha (\sqrt{-g} \nabla^{[\beta} A^{\alpha]}) = \mu_0 J^\beta$

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Dirac notation in Quantum Mechanics

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

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

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

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

Examples

▶ **Classical Mechanics**

▶ **Quantum mechanics**

▶ **Relativity**

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Examples

▼ Classical Mechanics

▶ *Inertia tensor for a triatomic molecule*

▶ Quantum mechanics

▶ Relativity

Examples

▼ 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*

▶ 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 kd_[i,j] - Component(r_[k], i) Component(r_[k], j)), k = 1 .. N);

There are 2 particles

▼ Classical Mechanics

▼ *Inertia tensor for a triatomic molecule*

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$$InertiaTensor := \sum_{k=1}^N m_k \left(\|\vec{r}_k\|^2 \delta_{i,j} - (\vec{r}_k)_i (\vec{r}_k)_j \right) \tag{1.1.1.1}$$

There are 3 particles

> $N := 3$

▼ 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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> N := 3

$$N := 3 \tag{1.1.1.2}$$

Create an indexing function

> ~~T~~ := unapply(InertiaTensor, i, j)

$$IT := (i, j) \mapsto \sum_{k=1}^3 m_k \left(\|\vec{r}_k\|^2 \delta_{i,j} - (\vec{r}_k)_i (\vec{r}_k)_j \right) \quad (1.1.1.3)$$

The inertia tensor matrix

> $IT_Matrix := Matrix(3, IT)$

$$IT_Matrix := \begin{bmatrix} \sum_{k=1}^3 m_k \left(\|\vec{r}_k\|^2 - (\vec{r}_k)_1^2 \right) & \sum_{k=1}^3 \left(-m_k (\vec{r}_k)_1 (\vec{r}_k)_2 \right) & \sum_{k=1}^3 \left(-m_k (\vec{r}_k)_1 (\vec{r}_k)_3 \right) \\ \sum_{k=1}^3 \left(-m_k (\vec{r}_k)_1 (\vec{r}_k)_2 \right) & \sum_{k=1}^3 m_k \left(\|\vec{r}_k\|^2 - (\vec{r}_k)_2^2 \right) & \sum_{k=1}^3 \left(-m_k (\vec{r}_k)_2 (\vec{r}_k)_3 \right) \\ \sum_{k=1}^3 \left(-m_k (\vec{r}_k)_1 (\vec{r}_k)_3 \right) & \sum_{k=1}^3 \left(-m_k (\vec{r}_k)_2 (\vec{r}_k)_3 \right) & \sum_{k=1}^3 m_k \left(\|\vec{r}_k\|^2 - (\vec{r}_k)_3^2 \right) \end{bmatrix} \quad (1.1.1.4)$$

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

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

$$position := \vec{r}_k = \vec{R}_k - \vec{R}_{CM} \quad (1.1.1.5)$$

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

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

$$IT_Matrix := \begin{bmatrix} \sum_{k=1}^3 (-m_k (\vec{r}_k)_1 (\vec{r}_k)_2) & \sum_{k=1}^3 m_k (\|\vec{r}_k\|^2 - (\vec{r}_k)_2^2) & \sum_{k=1}^3 (-m_k (\vec{r}_k)_2 (\vec{r}_k)_3) \\ \sum_{k=1}^3 (-m_k (\vec{r}_k)_1 (\vec{r}_k)_3) & \sum_{k=1}^3 (-m_k (\vec{r}_k)_2 (\vec{r}_k)_3) & \sum_{k=1}^3 m_k (\|\vec{r}_k\|^2 - (\vec{r}_k)_3^2) \end{bmatrix} \quad (1.1.1.4)$$

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

> R_[1] := -\frac{a}{2} i;

$$\vec{R}_1 := -\frac{a \hat{i}}{2} \quad (1.1.1.6)$$

> R_[2] := h k

$$\vec{R}_2 := h \hat{k} \quad (1.1.1.7)$$

> R_[3] := \frac{a}{2} i

> $R_{[2]} := h_k$

$$\vec{R}_2 := h \hat{k} \tag{1.1.1.7}$$

> $R_{[3]} := \frac{a}{2} i$

$$\vec{R}_3 := \frac{a \hat{i}}{2} \tag{1.1.1.8}$$

Two masses are equal

> $m_3 := m[1]$

$$m_3 := m_1 \tag{1.1.1.9}$$

The "center of mass"

> $R_{[CM]} := \text{Sum}(m[j] R_{[j]}, j = 1 .. N) / \text{Sum}(m[j], j = 1 .. N);$

$$\vec{R}_{CM} := \frac{\sum_{j=1}^3 m_j \vec{R}_j}{\sum_{j=1}^3 m_j} \tag{1.1.1.10}$$

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

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

$$> R_{[1]} := -\frac{a}{2} \hat{i};$$

$$\vec{R}_1 := -\frac{a \hat{i}}{2} \tag{1.1.1.6}$$

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$$\vec{R}_2 := h \hat{k} \tag{1.1.1.7}$$

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

$$\vec{R}_{CM} := \frac{m_2 h \hat{k}}{2 m_1 + m_2} \tag{1.1.1.11}$$

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

> $\text{seq}(\text{eval}(\text{position}, k = j), j = 1 .. N) \quad \mathbb{I}$

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

> $\text{IT_answer} := \text{simplify}(\text{eval}(\text{value}(\text{IT_Matrix}), [??]))$

>

$$\vec{R}_3 := \frac{a}{2} \tag{1.1.1.8}$$

Two masses are equal

```
> m3 := m[1]
```

$$m_3 := m_1 \tag{1.1.1.9}$$

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

$$\vec{R}_{CM} := \frac{m_2 h \hat{k}}{2 m_1 + m_2} \tag{1.1.1.11}$$

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

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

> R_[2] := h_k

$$\vec{R}_2 := h \hat{k} \tag{1.1.1.7}$$

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

$$\vec{R}_3 := \frac{a \hat{i}}{2} \tag{1.1.1.8}$$

Two masses are equal

> m_3 := 2 m[1]

$$m_3 := m_1 \tag{1.1.1.9}$$

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$$\vec{R}_{CM} := \frac{\sum_{j=1}^3 m_j \vec{R}_j}{\sum_{j=1}^3 m_j} \tag{1.1.1.10}$$

$$IT_answer := \begin{bmatrix} 0 & \frac{m_1 (8 m_1 a^2 + 3 a^2 m_2 + 12 m_2 h^2)}{4 (3 m_1 + m_2)} & 0 \\ \frac{m_1 a m_2 h}{2 (3 m_1 + m_2)} & 0 & \frac{m_1 a^2 (8 m_1 + 3 m_2)}{4 (3 m_1 + m_2)} \end{bmatrix} \quad (1.1.1.13)$$

>

▼ Quantum mechanics

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

- > restart; with(Physics) : interface(imaginaryunit = i) :
- > Setup(spaceindices = lowercase latin)

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

> Define(L, r, p)


```
> restart; with(Physics) : interface(imaginaryunit = i) :
> Setup(spaceindices = lowercaselatin)
[spaceindices = lowercaselatin] (2.1.1)
```

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,  $\gamma_\mu$ ,  $\sigma_\mu$ ,  $\partial_\mu$ ,  $g_{\mu, \nu}$ ,  $\delta_{\mu, \nu}$ ,  $\epsilon_{\alpha, \beta, \mu, \nu}$ } (2.1.2)
```

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})
[algebrarules = { [p_j, p_k]_ = 0, [r_j, p_k]_ = i  $\delta_{j, k}$ , [r_j, r_k]_ = 0 }, quantumoperators = {L, p, r}] (2.1.3)
```

Verify how these algebra rules work:

```
> %Commutator(r[j], p[k])
[r_j, p_k]_ (2.1.4)
```

```
> value(%)
```

$$\begin{aligned}
 &= i \text{KroneckerDelta}[j, k], \%Commutator(r[j], r[k]) = 0) \\
 &\left[\text{algebrarules} = \left\{ [p_j, p_k]_- = 0, [r_j, p_k]_- = i \delta_{j,k}, [r_j, r_k]_- = 0 \right\}, \text{quantumoperators} = \{L, p, r\} \right] \quad (2.1.3)
 \end{aligned}$$

Verify how these algebra rules work:

> `%Commutator(r[j], p[k])`

$$[r_j, p_k]_- \quad (2.1.4)$$

> `value(%)`

$$i \delta_{j,k} \quad (2.1.5)$$

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

$$[r_j, r_k]_- = 0 \quad (2.1.6)$$

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

$$[p_j, p_k]_- = 0 \quad (2.1.7)$$

We want to verify that if

> `L[j] = ep_[j, k, m] r[k] p[m]`

$$L_j = r_k p_m \epsilon_j^{k,m} \quad (2.1.8)$$

then

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

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

$$[r_j, p_k]_- \tag{2.1.4}$$

> value(%)

$$i \delta_{j, k} \tag{2.1.5}$$

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

$$[r_j, r_k]_- = 0 \tag{2.1.6}$$

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

$$[p_j, p_k]_- = 0 \tag{2.1.7}$$

We want to verify that if

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

$$L_j = r_k p_m \epsilon_j^{k, m} \tag{2.1.8}$$

then

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

$$rule := [L_j, L_k]_- = i \epsilon_{j, k, m} L^m \tag{2.1.9}$$

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

> Library:-SubstituteTensor((2.1.8), rule)

$$[r_j, r_k]_- = 0 \tag{2.1.6}$$

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

$$[p_j, p_k]_- = 0 \tag{2.1.7}$$

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$$[r_a p_m \epsilon_j^{a, m}, r_b p_c \epsilon_k^{b, c}]_- = i \epsilon_{j, k, m} r_a p_b \epsilon^{m, a, b} \tag{2.1.10}$$

> Simplify((2.1.10))

$$-i r_k p_j + i r_j p_k = -i r_k p_j + i r_j p_k \tag{2.1.11}$$

Or one step at a time,

> expand((2.1.10))

Library:-SubstituteTensor ((2.1.6), rule)

$$\left[r_a p_m \epsilon_j^{a,m}, r_b p_c \epsilon_k^{b,c} \right]_- = i \epsilon_{j,k,m} r_a p_b \epsilon^{m,a,b} \quad (2.1.10)$$

> *Simplify*((2.1.10))

$$-i r_k p_j + i r_j p_k = -i r_k p_j + i r_j p_k \quad (2.1.11)$$

Or one step at a time,

> *expand*((2.1.10))

$$\epsilon_j^{a,m} \epsilon_k^{b,c} r_a p_m r_b p_c - \epsilon_j^{a,m} \epsilon_k^{b,c} r_b p_c r_a p_m = i \epsilon_{j,k,m} \epsilon^{a,b,m} r_a p_b \quad (2.1.12)$$

> *Simplify*((2.1.12))

ⓘ

$$-i r_k p_j + i r_j p_k = -i r_k p_j + i r_j p_k \quad (2.1.13)$$

> [

- ▶ ***Quantization of the energy of a particle in a magnetic field***
- ▶ ***The field equations for a quantum system of identical particles***
- ▶ ***Unitary Operators in Quantum Mechanics***

$\vec{k}^T \vec{j}$ $\vec{j}^T \vec{k}$ $\vec{k}^T \vec{j}$ $\vec{j}^T \vec{k}$

>

▼ *Quantization of the energy of a particle in a magnetic field*

Show that the energy of a particle in a 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 , a are creation and annihilation operators.

> `restart; with(Physics) : with(Physics[Vectors]) : interface(imaginaryunit = i) :`

> `Setup(hermitianoperators = { H, Pi_-, Pi, A, A_-, L, p_-, p, x, y, z }, quantumoperators = { a }, realobjects = { c, h, q, k, B, m, omega_c })`

$$\left[\text{hermitianoperators} = \{ \vec{\Pi}, A, \vec{A}, H, L, \Pi, p, \vec{p}, x, y, z \}, \text{quantumoperators} = \{ \vec{\Pi}, A, \vec{A}, H, L, \Pi, a, p, \vec{p}, x, y, z \}, \text{(2.2.1)} \right.$$

$$\left. \text{realobjects} = \{ \hbar, B, \hat{i}, \hat{j}, \hat{k}, \hat{\phi}, \hat{r}, \hat{\rho}, \hat{\theta}, c, k, m, \phi, q, r, \rho, \theta, x, y, z, \omega_c \} \right]$$

> `CompactDisplay(A(x, y), A_-(x, y))`

$$> H = \frac{\left(p_- - \frac{q}{c} \cdot A_-(x, y) \right)^2}{2 \cdot m}$$

$$H = \frac{\left(\vec{p} - \frac{q \vec{A}}{c} \right)^2}{2 m} \tag{2.2.3}$$

Let's introduce the Hermitian operator $\vec{\Pi}$

$$> \Pi_- = p_- - \frac{q}{c} \cdot A_-(x, y)$$

$$\vec{\Pi} = \vec{p} - \frac{q \vec{A}}{c} \tag{2.2.4}$$

> *substitute*((rhs = lhs) ((2.2.4)), (2.2.3))

$$H = \frac{\vec{\Pi}^2}{2 m} \tag{2.2.5}$$

Derive now the commutation rules $[\Pi_x, \Pi_y]$ for the components of $\vec{\Pi}$ taking into account the commutator rules between position and momentum:

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

> Component((2.2.10), 1)

$$\Pi_x = p_x - \frac{q A_x}{c} \tag{2.2.11}$$

> Component((2.2.10), 2)

$$\Pi_y = p_y - \frac{q A_y}{c} \tag{2.2.12}$$

> %Commutator((2.2.11), (2.2.12))

$$\left[\Pi_x = p_x - \frac{q A_x}{c}, \Pi_y = p_y - \frac{q A_y}{c} \right] \tag{2.2.13}$$

> value((2.2.13))

$$\left[\Pi_x, \Pi_y \right] = -\frac{q [p_x, A_y]}{c} - \frac{q \left([A_x, p_y] - \frac{q [A_x, A_y]}{c} \right)}{c} \tag{2.2.14}$$

We need to specify the gauge to compute the commutators that involve $\vec{A}(x, y)$. In Coulomb's gauge, the following vector potential gives the chosen magnetic field $\vec{B} = B \hat{k}$

> $A(x, y) = -\frac{B \cdot y}{c} \cdot i + \frac{B \cdot x}{c} \cdot j;$

between position and momentum:

$$\begin{aligned}
 &> \text{Setup}\left(\left\{\left[x, p_x\right]_- = i \hbar, \left[x, p_y\right]_- = 0, \left[y, x\right]_- = 0, \left[y, p_x\right]_- = 0, \left[y, p_y\right]_- = i \hbar, \left[p_y, p_x\right]_- = 0\right\}\right) \\
 &\quad \left[\text{algebrarules} = \left\{\left[x, p_x\right]_- = i \hbar, \left[x, p_y\right]_- = 0, \left[y, x\right]_- = 0, \left[y, p_x\right]_- = 0, \left[y, p_y\right]_- = i \hbar, \left[p_y, p_x\right]_- = 0\right\}\right] \quad (2.2.6)
 \end{aligned}$$

Express then these vectors in components

$$\begin{aligned}
 &> p_- = p[x] \cdot _i + p[y] \cdot _j \\
 &\qquad\qquad\qquad \vec{p} = \hat{i} p_x + \hat{j} p_y \quad (2.2.7)
 \end{aligned}$$

$$\begin{aligned}
 &> A_-(x, y) = A[x](x, y) \cdot _i + A[y](x, y) \cdot _j \\
 &\qquad\qquad\qquad \vec{A} = \hat{i} A_x + \hat{j} A_y \quad (2.2.8)
 \end{aligned}$$

$$\begin{aligned}
 &> \Pi_- = \Pi[x] \cdot _i + \Pi[y] \cdot _j \\
 &\qquad\qquad\qquad \vec{\Pi} = \hat{i} \Pi_x + \hat{j} \Pi_y \quad (2.2.9)
 \end{aligned}$$

$$\begin{aligned}
 &> \text{substitute}\left(\left[(2.2.7), (2.2.8), (2.2.9)\right], (2.2.4)\right) \\
 &\qquad\qquad\qquad \hat{i} \hat{\Pi}_x + \hat{j} \hat{\Pi}_y = \hat{i} p_x + \hat{j} p_y - \frac{q \left(\hat{i} A_x + \hat{j} A_y\right)}{c} \quad (2.2.10)
 \end{aligned}$$

$$\begin{aligned}
 &> \text{Component}\left((2.2.10), 1\right) \\
 &\qquad\qquad\qquad \Pi_x = p_x - \frac{q A_x}{c} \quad (2.2.11)
 \end{aligned}$$

Show that the energy of a particle in a 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, a are creation and annihilation operators.

- > `restart with(Physics) : with(Physics[Vectors]) : interface(imaginaryunit = i) :`
- > `Setup(hermitianoperators = { H, Pi_, Pi, A, A_, L, p_, p, x, y, z }, quantumoperators = { a }, realobjects = { c, h, q, k, B, m, omega_c })`
- `[hermitianoperators = { Pi, A, A, H, L, Pi, p, p, x, y, z }, quantumoperators = { Pi, A, A, H, L, Pi, a, p, p, x, y, z }, (2.2.1)`
`realobjects = { h, B, i, j, k, phi, r, rho, theta, c, k, m, phi, q, r, rho, theta, x, y, z, omega_c }]`
- > `CompactDisplay(A(x, y), A_(x, y))`
 $A(x, y)$ will now be displayed as A
 $\vec{A}(x, y)$ will now be displayed as \vec{A} (2.2.2)

$$\left[\Pi_x = p_x - \frac{q A_x}{c}, \Pi_y = p_y - \frac{q A_y}{c} \right] \quad (2.2.13)$$

> value((2.2.13))

$$\left[\Pi_x, \Pi_y \right] = -\frac{q [p_x, A_y]}{c} - \frac{q \left([A_x, p_y] - \frac{q [A_x, A_y]}{c} \right)}{c} \quad (2.2.14)$$

We need to specify the gauge to compute the commutators that involve $\vec{A}(x, y)$. In Coulomb's gauge, the following vector potential gives the chosen magnetic field $\vec{B} = B \hat{k}$

$$A(x, y) = -\frac{B \cdot y}{2} \cdot i + \frac{B \cdot x}{2} \cdot j \quad \text{I}$$

Verify

> Divergence(??)

> Curl(??)

Express the left-hand side of ?? in terms of the components of A and recompute $\left[\Pi_x, \Pi_y \right]$

> substitute((2.2.8), ??)

> convert(??, setofequations)

> substitute(??, (2.2.14))

> ??

> Setup(2.2.20)

$$algebrarules = \left\{ [x, p_x]_- = i \hbar, [x, p_y]_- = 0, [y, x]_- = 0, [y, p_x]_- = 0, [y, p_y]_- = i \hbar, [\Pi_x, \Pi_y]_- = \frac{i q B \hbar}{c}, [p_y, p_x]_- = 0 \right\} \quad (2.2.22)$$

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

$$a = \frac{\sqrt{c} \sqrt{2} (\Pi_x + i \Pi_y)}{2 \sqrt{\hbar q B}} \quad (2.2.23)$$

> (2.2.23)*

$$a^\dagger = \frac{\sqrt{c} \sqrt{2} (\Pi_x - i \Pi_y)}{2 \sqrt{\hbar q B}} \quad (2.2.24)$$

Verify the normalization of this definition

> Commutator(2.2.23, 2.2.24)

$$[a, a^\dagger]_- = 1 \quad (2.2.25)$$

Express the Hamiltonian in terms of a, a^\dagger . For that purpose, multiply equations (2.2.24) and (2.2.23)

> ((2.2.24) . (2.2.23))

$$a^\dagger a = -\frac{1}{2} + \frac{c \Pi_y^2}{2 \hbar \omega_c m} + \frac{c \Pi_x^2}{2 \hbar \omega_c m} \quad (2.2.27)$$

Introduce the angular frequency

$$> \omega_c = \frac{q \cdot B}{m}$$

$$\omega_c = \frac{q B}{m} \quad (2.2.28)$$

> isolate((2.2.28), B)

$$B = \frac{\omega_c m}{q} \quad (2.2.29)$$

> expand(substitute((2.2.29), (2.2.27)))

$$a^\dagger a = -\frac{1}{2} + \frac{c \Pi_y^2}{2 \hbar \omega_c m} + \frac{c \Pi_x^2}{2 \hbar \omega_c m} \quad (2.2.30)$$

Compare now this formula with the Hamiltonian:

> (2.2.9), (2.2.5)

$$\vec{\Pi} = \hat{i} \Pi_x + \hat{j} \Pi_y, H = \frac{\vec{\Pi}^2}{2 m} \quad (2.2.31)$$

> expand(substitute((2.2.9), (2.2.5)))

$$\left[\Pi_x = p_x - \frac{q A_x}{c}, \Pi_y = p_y - \frac{q A_y}{c} \right] \quad (2.2.13)$$

> value((2.2.13))

$$\left[\Pi_x, \Pi_y \right] = -\frac{q [p_x, A_y]}{c} - \frac{q \left([A_x, p_y] - \frac{q [A_x, A_y]}{c} \right)}{c} \quad (2.2.14)$$

We need to specify the gauge to compute the commutators that involve $\vec{A}(x, y)$. In Coulomb's gauge, the following vector potential gives the chosen magnetic field $\vec{B} = B \hat{k}$

$$\begin{aligned} > A(x, y) = -\frac{B \cdot y}{2} \cdot i + \frac{B \cdot x}{2} \cdot j; \\ \vec{A} = -\frac{1}{2} B \hat{i} y + \frac{1}{2} B \hat{j} x \end{aligned} \quad (2.2.15)$$

Verify

> Divergence((2.2.15))

$$\nabla \cdot \vec{A} = 0 \quad (2.2.16)$$

> Curl((2.2.15))

$$\nabla \times \vec{A} = B \hat{k} \quad (2.2.17)$$

Express the left hand side of (2.2.14) in terms of the components of A and recompute [Pi_x, Pi_y]

vector potential gives the chosen magnetic field $B = B \hat{k}$

> $A(x, y) = -\frac{B \cdot y}{2} \cdot \hat{i} + \frac{B \cdot x}{2} \cdot \hat{j};$

$$\vec{A} = -\frac{1}{2} B \hat{i}_y + \frac{1}{2} B \hat{j}_x \tag{2.2.15}$$

Verify

> *Divergence*((2.2.15))

$$\nabla \cdot \vec{A} = 0 \tag{2.2.16}$$

> *Curl*((2.2.15))

$$\nabla \times \vec{A} = B \hat{k} \tag{2.2.17}$$

Express the left-hand side of (2.2.15) in terms of the components of A and recompute $[\Pi_x, \Pi_y]$

> *substitute*((2.2.8), (2.2.15))

$$\hat{i} A_x + \hat{j} A_y = -\frac{1}{2} B \hat{i}_y + \frac{1}{2} B \hat{j}_x \tag{2.2.18}$$

> *convert*((2.2.18), setofequations)

$$\left\{ A_x = -\frac{B y}{2}, A_y = \frac{B x}{2} \right\} \tag{2.2.19}$$

> *substitute*((2.2.19), (2.2.14))

> $A(x, y) = -\frac{B \cdot y}{2} \cdot i + \frac{B \cdot x}{2} \cdot j;$

$$\vec{A} = -\frac{1}{2} B \hat{i}_y + \frac{1}{2} B \hat{j}_x \tag{2.2.15}$$

Verify

> *Divergence*((2.2.15))

$$\nabla \cdot \vec{A} = 0 \tag{2.2.16}$$

> *Curl*((2.2.15))

$$\nabla \times \vec{A} = B \hat{k} \tag{2.2.17}$$

Express the left-hand side of (2.2.15) in terms of the components of A and recompute $[\Pi_x, \Pi_y]$

> *substitute*((2.2.8), (2.2.15))

$$\hat{i} A_x + \hat{j} A_y = -\frac{1}{2} B \hat{i}_y + \frac{1}{2} B \hat{j}_x \tag{2.2.18}$$

> *convert*((2.2.18), setofequations)

$$\left\{ A_x = -\frac{B y}{2}, A_y = \frac{B x}{2} \right\} \tag{2.2.19}$$

> *substitute*((2.2.19), (2.2.14))

$$\left(\dots, q \left[-\frac{B y}{2}, \frac{B x}{2} \right] \right)$$

> simplify((2.2.32), {(2.2.30)}, { Π_x^2 })

$$H = \frac{2 a^\dagger a \hbar \omega_c m + \hbar \omega_c m}{2 c m} \quad (2.2.33)$$

> simplify((2.2.33), size)

$$H = \frac{\hbar \omega_c (2 a^\dagger a + 1)}{2 c} \quad (2.2.34)$$

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

>

▼ *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).

I

► **Solution**

> $E := \frac{1}{2m} \text{Norm}(\% \text{Gradient}(\Psi)) + V(x, y, z, t) \text{abs}(\Psi) + \frac{G}{2} \text{abs}(\Psi)^2 ;$

$$E := \frac{\hbar^2 \|\nabla \Psi\|^2}{2m} + V|\Psi|^2 + \frac{G|\Psi|^4}{2} \tag{2.3.1.2}$$

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

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

The Lagrangian density L in terms of the Energy E

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

$$L := \frac{i \hbar (\bar{\Psi} \Psi_t - \Psi \bar{\Psi}_t)}{2} - \frac{\hbar^2 \|\nabla \Psi\|^2}{2m} - V|\Psi|^2 - \frac{G|\Psi|^4}{2} \tag{2.3.1.3}$$

Construct the action and equate to zero the functional derivative

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

$$\left(\frac{\delta}{\delta \Psi} \right) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{i \hbar (\bar{\Psi} \Psi_t - \Psi \bar{\Psi}_t)}{2} - \frac{\hbar^2 \|\nabla \Psi\|^2}{2m} - V|\Psi|^2 - \frac{G|\Psi|^4}{2} \right) dx dy dz dt = 0 \tag{2.3.1.4}$$

> (2.3.1.4)

> (2.3.1.4)

$$\frac{\hbar^2 \bar{\psi}_{x,x} + \bar{\psi}_{y,y} \hbar^2 + \hbar^2 \bar{\psi}_{z,z} - 2 (G \bar{\psi}^2 \psi + i \bar{\psi}_t \hbar + \bar{\psi} V) m}{2 m} = 0 \tag{2.3.1.5}$$

Make the Laplacian explicit

> (Laplacian = %Laplacian) (Psi)

$$\psi_{x,x} + \psi_{y,y} + \psi_{z,z} = \nabla^2 \psi \tag{2.3.1.6}$$

> simplify(conjugate((2.3.1.5)), {(2.3.1.6)})

$$\frac{\hbar^2 \nabla^2 \psi}{2 m} + \frac{-2 G \bar{\psi} \psi^2 m + 2 i \hbar \psi_t m - 2 \psi V m}{2 m} = 0 \tag{2.3.1.7}$$

The standard form of the Gross–Pitaevskii equation:

> i \hbar isolate((2.3.1.7), diff(Psi, t))

$$i \psi_t \hbar = \frac{-\frac{\hbar^2 \nabla^2 \psi}{2} + G \bar{\psi} \psi^2 m + \psi V m}{m} \tag{2.3.1.8}$$

> collect(convert(expand((2.3.1.8)), abs), psi)

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

(2.3.1.1)

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

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

$$E := \frac{\hbar^2 \|\nabla\Psi\|^2}{2m} + V|\Psi|^2 + \frac{G|\Psi|^4}{2}$$

(2.3.1.2)

$\Psi(x, y, z, t)$ 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, h, G, V(x, y, z, t)}) :

The Lagrangian density L in terms of the Energy E

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

- ▶ 2) Properties of unitary operators
- ▶ 3) Schrödinger equation and unitary transform
- ▶ 4) Galilean transform and spatial translation operators
- ▶ 5) Basis change and Dirac notation

I

▼ Relativity

- ▶ *Maxwell equations departing from the 4-dimensional Action for Electrodynamics*
- ▶ *A problem in General Relativity*

- ▶ 2) Properties of unitary operators
- ▶ 3) Schrödinger equation and unitary transform
- ▶ 4) Galilean transform and spatial translation operators
- ▶ 5) Basis change and Dirac notation

▼ Relativity

▼ *Maxwell equations departing from the 4-dimensional Action for Electrodynamics*

Maxwell equations result from equation to zero the functional derivative of the Action with respect to the 4-D potential

A

► 5) Basis change and Dirac notation

▼ **Relativity**

▼ *Maxwell equations departing from the 4-dimensional Action for Electrodynamics*

Maxwell equations result from equation to zero the functional derivative of the Action with respect to the 4-D potential

$$A_{\mu}$$

- > restart; with(Physics) :
- > Coordinates(X)

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));

Equates to 0 the functional derivative of the corresponding Action

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

> $F[\text{mu}, \text{nu}] := d_{[\text{mu}}(A[\text{nu}](X)) - d_{[\text{nu}}(A[\text{mu}](X));$
 $F_{\mu, \nu} := \partial_{\mu}(A_{\nu}) - (\partial_{\nu}(A_{\mu}))$ (3.1.4)

Equate to 0 the functional derivative of the corresponding Action

> $'Fundiff'(Intc(F[\text{mu}, \text{nu}]^2, X), A[\text{rho}]) = 0$
 $\left(\frac{\delta}{\delta A_{\rho}}\right) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\partial_{\mu}(A_{\nu}) - (\partial_{\nu}(A_{\mu})))^2 dx1 dx2 dx3 dx4 = 0$ (3.1.5)

> (3.1.5)
 $\left(2 \left(\partial_{\mu} \left(\partial_{\nu} \left(A^{\nu}\right)\right)\right) - 2 \square \left(A_{\mu}\right)\right) g^{\mu, \rho} + \left(-2 \square \left(A_{\nu}\right) + 2 \left(\partial_{\mu} \left(\partial_{\nu} \left(A^{\mu}\right)\right)\right)\right) g^{\nu, \rho} = 0$ (3.1.6)

Simplify the contracted spacetime indices

> $Simplify((3.1.6))$
 $-4 \square \left(A^{\rho}\right) + 4 \left(\partial_{\mu} \left(\partial^{\rho} \left(A^{\mu}\right)\right)\right) = 0$ (3.1.7)

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

> $OFF; convert(Library:-TensorComponents((3.1.7)), diff)$

$$\begin{aligned}
 & -4 \left(\frac{\partial^2}{\partial x_3 \partial x_4} A^4(X) \right) = 0, 4 \left(\frac{\partial^2}{\partial x_1^2} A^4(X) \right) + 4 \left(\frac{\partial^2}{\partial x_2^2} A^4(X) \right) + 4 \left(\frac{\partial^2}{\partial x_3^2} A^4(X) \right) \\
 & + 4 \left(\frac{\partial^2}{\partial x_1 \partial x_4} A^1(X) \right) + 4 \left(\frac{\partial^2}{\partial x_2 \partial x_4} A^2(X) \right) + 4 \left(\frac{\partial^2}{\partial x_3 \partial x_4} A^3(X) \right) = 0
 \end{aligned}$$

>

▼ *A problem in General Relativity*

Problem: for the spacetime metric,

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

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^{β} is the Ricci tensor, \mathcal{D} is the covariant derivative

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

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

b) Compute the components of $W_{\alpha}^{\beta} \equiv$ the traceless part of Z_{α}^{β} of item **a)**

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

Background: The equations of items **a)** and **b)** appear in a paper from February/2013, "[Withholding Potentials, Absence of Ghosts and Relationship between Minimal Dilatonic Gravity and f\(R\) Theories](#)", by P. Fiziev.

>

$$I_{\alpha, \beta} = \begin{vmatrix} 0 & 0 & 8 r^2 \sin(\theta)^2 \pi & 0 \\ 0 & 0 & 0 & 8 e^{v(r)} \pi \epsilon \end{vmatrix}$$

b) Compute the components of $W_{\alpha}^{\beta} \equiv$ the traceless part of Z_{α}^{β} of item **a)**

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

Background: The equations of items **a)** and **b)** appear in a 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)*

```
Maple 18 File Edit View Insert Format Table Drawing Plot Spreadsheet Tools Window Help 83% Tue Oct 7 10:55
on background.mw
> g_[ ] I
> g_[ ~mu,~nu, matrix ]
> Christoffel[ ~2, mu, nu, matrix ]
> Ricci[ ]
> Riemann[ ~1, mu, nu,~2, matrix ]
>
```

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$$R_{\mu, \nu} = \begin{bmatrix} \frac{-v_r r + v_r \lambda_r r - 2 v_{r,r} r + 4 \lambda_r}{4 r}, 0, 0, 0 \\ 0, 1 + \frac{(-v_r r + \lambda_r r - 2) e^{-\lambda}}{2}, 0, 0 \\ 0, 0, -\frac{\sin(\theta)^2 (-2 + (v_r r - \lambda_r r + 2) e^{-\lambda})}{2}, 0 \\ 0, 0, 0, \frac{(2 v_{r,r} r + v_r (v_r r - \lambda_r r + 4)) e^{-\lambda + \nu}}{4 r} \end{bmatrix} \quad (4)$$

> Riemann[~1, mu, nu, ~2, matrix]

$$R_{\mu, \nu}^1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ -\frac{e^{-\lambda} \lambda_r}{2 r} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (5)$$

$$\left[\begin{array}{l} 8 r^2 \dots \\ -4 \dots \end{array} \right] e^{-\lambda} - 4 \Phi + (-16 \epsilon - 16) \pi r^2 \dots 0 \left. \right] \\ \left[\begin{array}{l} 0, 0, 0, -\frac{1}{8 r^2} \left(\left(\left(-2 \Phi_{r,r} r^2 - 2 v_{r,r} \Phi r^2 - v_r^2 \Phi r^2 + r (\lambda_r \Phi r + 3 \Phi_r r - 4 \Phi) v_r + r (\Phi_r r \right. \right. \right. \\ \left. \left. \left. - 4 \Phi) \lambda_r - 4 \Phi_r r + 4 \Phi \right) e^{-\lambda + v} - 48 \left(\frac{\Phi}{12} + (\epsilon + 1) \pi r^2 \right) e^v \right) e^{-v} \right) \right] \end{array} \right]$$

>
 ▼ **c) An exact solution for the nonlinear system of differential equations conformed by the components of W_{α}^{β}**

Create an ODE system with the nonzero components of W_{μ}^{ν}

```
> ode_system := map(u -> rhs(u) = 0, rhs(W[mu,~nu, nonzero]))
> Case := simplify([PDEtools:-casesplit(ode_system)], size) :
```

There are three cases
 > nops(Case)

sol_subsystem

$$-\frac{1}{\sqrt{\pi(\epsilon+1)}} \left(\ln \left(\frac{(32\epsilon+32)\pi+4_C1}{\pi(\epsilon+1) \left(r \frac{\sqrt{(8\epsilon+8)\pi+_C1}}{\sqrt{\pi(\epsilon+1)}} _C2 - _C3 \right)^2} \right) \sqrt{\pi(\epsilon+1)} \right. \\ \left. + \ln(r) \left(\sqrt{(8\epsilon+8)\pi+_C1} - 2\sqrt{\pi(\epsilon+1)} \right) \right), \lambda = _C2$$

Specialize one of these constants using the constraint

> eval(constraint, sol_subsystem)

$$\left[e^{-C2} = -\frac{C1}{4(\epsilon+1)\pi} \right] \tag{3.2.3.7}$$

> solve((3.2.3.7), _C1)

$$\{ _C1 = -4 e^{-C2} \pi \epsilon - 4 e^{-C2} \pi \} \tag{3.2.3.8}$$

The exact solution

> solution := substitute((3.2.3.8), sol_subsystem)

The exact solution

> `solution := substitute((3.2.3.8), solsubsystem)`

$$\text{solution} := \left\{ \Phi = (-4 e^{-C2} \pi \epsilon - 4 e^{-C2} \pi) r^2, v = \right. \tag{3.2.3.9}$$

$$\left. -\frac{1}{\sqrt{\pi(\epsilon+1)}} \left(\ln \left(\frac{(32\epsilon+32)\pi - 16e^{-C2}\pi\epsilon - 16e^{-C2}\pi}{\left(\pi(\epsilon+1) \left(r \frac{\sqrt{(8\epsilon+8)\pi - 4e^{-C2}\pi\epsilon - 4e^{-C2}\pi}}{\sqrt{\pi(\epsilon+1)}} \right) \right)^2} \right) \sqrt{\pi(\epsilon+1)} \right. \right.$$

$$\left. \left. + \ln(r) \left(\sqrt{(8\epsilon+8)\pi - 4e^{-C2}\pi\epsilon - 4e^{-C2}\pi} - 2\sqrt{\pi(\epsilon+1)} \right) \right), \lambda = -C2 \right\}$$

Verifying this result

> `odetest(solution, odesystem)`

{0}

(3.2.3.10)

> [