Amplitude functions and properties of the H atom from the Dirac equation in spherical polar coordinates

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```
> restart:
```

Whereas the conventional wave equation contains partial derivatives in spatial and time variables of both second order, Schroedinger's temporally dependent equation has the form of a diffusion equation; it fails to conform to a relativistic requirement because it contains spatial derivatives of second order whereas a temporal derivative of first order, as Schroedinger recognised at the time of producing this equation. For comparison with the shapes of the surfaces of amplitude functions from the solution of Schroedinger's temporally independent equations, we present here the solutions to Dirac's equation for the hydrogen atom that contains derivatives with respect to spatial and temporal variables both of first order, but the resulting amplitude functions must become vectors with four components. To form these amplitude functions we recall four Pauli spin matrices, as follows.

```
> sigma[0] := <<1|0>,<0|1>>;
  sigma[1] := sigma[x] = <<0|1>,<1|0>>;
  sigma[2] := sigma[y] = <<0|-I>,<I|0>>;
  sigma[3] := sigma[z] = <<1|0>,<0|-1>>;
```

$$\sigma_0 := \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\sigma_1 := \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_2 := \sigma_y = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}$$

$$\sigma_3 := \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

As introduced in exercise *e6.113*, these complex matrices are hermitian, such that a transpose of each matrix is equal to a matrix of the complex conjugates of its elements, unitary, such that its conjugate transpose is its inverse, and involutory, such that $\sigma_1^{\;2} = \sigma_2^{\;2} = \sigma_3^{\;2} = -i\,\sigma_1\,\sigma_2\,\sigma_3 = \mathbf{1}$, the unit mitrix. With these Pauli matrices as submatrices, we construct Dirac's dimensionless velocity operators, as follows; each product with speed of light c generates a component of velocity. Although these Dirac matrices contain the Pauli matrices as sub-matrices, this condition is fortuitous; the only matrices of order 4 for which the conditions of anticommuting and unit squares are fulfilled are those with exactly the stated compositions. Although the conventional notation for these velocity and aspect matrices comprises α and β, respectively, here we use α1 and β1 to leave α free for use below as the fundamental physical constant known as the fine-structure constant.

```
> alpha1[x] := <<0|0|0|1>,<0|0|1|0>,<0|1|0|0>,<1|0|0|0>>;
  alpha1[y] := <<0|0|0|-I>,<0|0|I|0>,<0|-I|0|0>,<I|0|0|0>>;
```

```
alpha1[z] := <<0|0|1|0>,<0|0|0|-1>,<1|0|0|0>,<0|-1|0|0>>;
beta1 := <<1|0|0|0>,<0|1|0|0>,<0|0|-1|0>,<0|0|0|-1>>;     #
aspect
```

$$\alpha 1_x := \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$$\alpha 1_y := \begin{bmatrix} 0 & 0 & 0 & -I \\ 0 & 0 & I & 0 \\ 0 & -I & 0 & 0 \\ I & 0 & 0 & 0 \end{bmatrix}$$

$$\alpha 1_z := \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

$$\beta 1 := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

Like the Pauli matrices, the squares of these Dirac matrices are unit matrices,

```
> 'alpha1[x].alpha1[x]' = alpha1[x].alpha1[x];
  'alpha1[y].alpha1[y]' = alpha1[y].alpha1[y];
  'alpha1[z].alpha1[z]' = alpha1[z].alpha1[z];
  'beta1.beta1' = beta1.beta1;
```

$$(\alpha 1_x) . (\alpha 1_x) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$(\alpha 1_y) . (\alpha 1_y) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$(\alpha 1_z) . (\alpha 1_z) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\beta 1 . \beta 1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

and the matrices anticommute such that $x\,y = -y\,x$, or the sum of these products in reverse order is zero; both the Pauli and Dirac matrices have these properties.

```
> 'alpha1[x]'.'alpha1[y]' + 'alpha1[y]'.'alpha1[x]' =
  alpha1[x].alpha1[y] + alpha1[y].alpha1[x];
```

$$((\alpha 1_x) \,.\, (\alpha 1_y)) + ((\alpha 1_y) \,.\, (\alpha 1_x)) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

```
> 'alpha1[x]'.'alpha1[z]' + 'alpha1[z]'.'alpha1[x]' =
  alpha1[x].alpha1[z] + alpha1[z].alpha1[x];
```

$$((\alpha 1_x) \,.\, (\alpha 1_z)) + ((\alpha 1_z) \,.\, (\alpha 1_x)) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

```
> 'alpha1[y]'.'alpha1[z]' + 'alpha1[z]'.'alpha1[y]' =
  alpha1[y].alpha1[z] + alpha1[z].alpha1[y];
```

$$((\alpha 1_y) \,.\, (\alpha 1_z)) + ((\alpha 1_z) \,.\, (\alpha 1_y)) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

```
> 'alpha1[x]'.'beta1' + 'beta1'.'alpha1[x]' = alpha1[x].beta1 +
  beta1.alpha1[x];
```

$$((\alpha 1_x) \,.\, \beta 1) + (\beta 1 \,.\, (\alpha 1_x)) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

```
> 'alpha1[y]'.'beta1' + 'beta1'.'alpha1[y]' = alpha1[y].beta1 +
  beta1.alpha1[y];
```

$$((\alpha 1_y) \,.\, \beta 1) + (\beta 1 \,.\, (\alpha 1_y)) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

```
> 'alpha1[z]'.'beta1' + 'beta1'.'alpha1[z]' = alpha1[z].beta1 +
  beta1.alpha1[z];
```

$$((\alpha 1_z) \,.\, \beta 1) + (\beta 1 \,.\, (\alpha 1_z)) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

To produce an energy of a system such as a hydrogen atom, Dirac formed an hamiltonian relation of this form, $H = -\alpha_x\, p_x\, c - \alpha_y\, p_y\, c - \alpha_z\, p_z\, c - \beta\, m_e\, c^2$, because its square leads to the relativistically correct equation for energy squared, $E^2 = {p_x}^2\, c^2 + {p_y}^2\, c^2 + {p_z}^2\, c^2 + {m_e}^2\, c^4$,

```
> E^2 = simplify((- alpha1[x]*p[x]*c - alpha1[y]*p[y]*c -
```

```
alpha1[z]*p[z]*c - beta1*m[e]*c^2)^2);
```

$$E^2 = \begin{bmatrix} c^2 (c^2 m_e^2 + p_x^2 + p_y^2 + p_z^2), 0, 0, 0 \\ 0, c^2 (c^2 m_e^2 + p_x^2 + p_y^2 + p_z^2), 0, 0 \\ 0, 0, c^2 (c^2 m_e^2 + p_x^2 + p_y^2 + p_z^2), 0 \\ 0, 0, 0, c^2 (c^2 m_e^2 + p_x^2 + p_y^2 + p_z^2) \end{bmatrix}$$

provided that the square of each operator α_x, α_y, α_z, β becomes unity and that a product of any two changes sign on multiplication in a reverse order; tests above prove that the specified Dirac matrices fulfil these conditions. On that basis, Dirac's system of equations for an electron of mass m_e in an electromagnetic field with scalar potential A_0 and vector potential $\underline{A} = (A_1, A_2, A_3)$ is expressible as

$$\left(p_0 \mathbf{I} + \sum_{j=1}^{3} \alpha_j p_j + \beta m_e c \right) \psi = 0,$$

in which $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)$ is a vector with four components, $\mathbf{I}$ is a unit matrix of order 4, α_j and β are the Dirac matrices specified above and p_j are momenta that become differential operators of space variables or time:

$$p_0 = \frac{i\,h}{2\,\pi\,c}\frac{\partial}{\partial t} + \frac{e}{c} A_0, \qquad p_j = -\frac{i\,h}{2\,\pi}\frac{\partial}{\partial x_j} + \frac{e}{c} A_j \quad \text{for } j = 1, 2, 3$$

For the particular case of a central field of force such as a coulombic potential energy, $A_0 = \frac{c}{e}$ $\mathrm{V}(r)$ and $A_j = 0$ for $j = 1, 2, 3$; for solutions periodic in time, p_0 becomes a parameter equal to $\frac{1}{c}$ times energy E. Assuming distances in unit $\frac{a_0}{Z}$, in which appear Bohr radius a_0 and atomic number Z, and eigenfunctions in terms of $\sqrt{\frac{Z^3}{\pi\,a_0^{\,3}}}$, Dirac's equation, independent of time, for an atom of proton number Z and only one electron is then

$$\left(E + \frac{Z\,e^2}{4\,\pi\,\varepsilon_0\,r} \right) \psi = i\,h\,c \left(\alpha_x \left(\frac{\partial}{\partial x} \right) + \alpha_y \left(\frac{\partial}{\partial y} \right) + \alpha_z \left(\frac{\partial}{\partial z} \right) \right) \psi - \beta\,m_e\,c^2\,\psi$$

in which appear $i = \sqrt{-1}$, electronic charge $-e$ and rest mass m_e, speed of light c, electric permittivity of free space ε_0, Planck constant h and energy eigenvalue E, with four Dirac matrices α_x, α_y, α_z, β; $m_e\,c^2$ represents the energy due to the rest mass of the electron. By dint of the occurrence of matrices α and β both of order 4, that equation implies four separate equations; each eigenfunction or amplitude function ψ must be a column vector with four components,

```
> psi = <psi[1],psi[2],psi[3],psi[4]>;
```

$$\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

which cannot be directly combined into a single algebraic formula. In contrast, as the square of the magnitude of ψ, the probability density $|\psi^2| = \psi^* \ \psi$ becomes a scalar product of a row vector, as the complex conjugate of ψ in which each component is a complex conjugate of the respective component of ψ,

```
> psi^`*` = <psi[1]^`*`|psi[2]^`*`|psi[3]^`*`|psi[4]^`*`>;
```

$$\psi^* = [\psi_1^* \quad \psi_2^* \quad \psi_3^* \quad \psi_4^*]$$

and the above column vector,

```
> psi^`* `*psi = '<psi[1]^`* `|psi[2]^`* `|psi[3]^`* `|psi[4]^`*
  `>' . <psi[1],psi[2],psi[3],psi[4]>;
```

$$\psi^* \ \psi = \langle \psi_1^* \mid \psi_2^* \mid \psi_3^* \mid \psi_4^* \rangle . \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

which evaluates to

```
> %;
```

$$\psi^* \ \psi = \psi_1^* \ \psi_1 + \psi_2^* \ \psi_2 + \psi_3^* \ \psi_3 + \psi_4^* \ \psi_4$$

which is simply a scalar quantity as a sum of the four indicated terms, each a product of a component of the vectorial eigenfunction with its complex conjugate.

We classify the eigenfunction or amplitude function of this Dirac equation independent of time in terms of four quantum numbers:

- energy quantum number n, which originated from experiment through the formulae of Balmer and Rydberg and which assumes values of positive integers; this quantum number can be replaced for all purposes of identification with a sum of radial quantum number k, that indicates the number of radial nodes in a particular component of the amplitude function, azimuthal quantum number l and unity, such that $n = k + l + 1$ as in the Schroedinger case in spherical polar coordinates, so that a state becomes identified as $|k+l+1, l, j, m\rangle$;

- azimuthal quantum number l, which assumes values of non-negative integers up to $n - 1$, but which is no longer a quantum number for angular momentum;

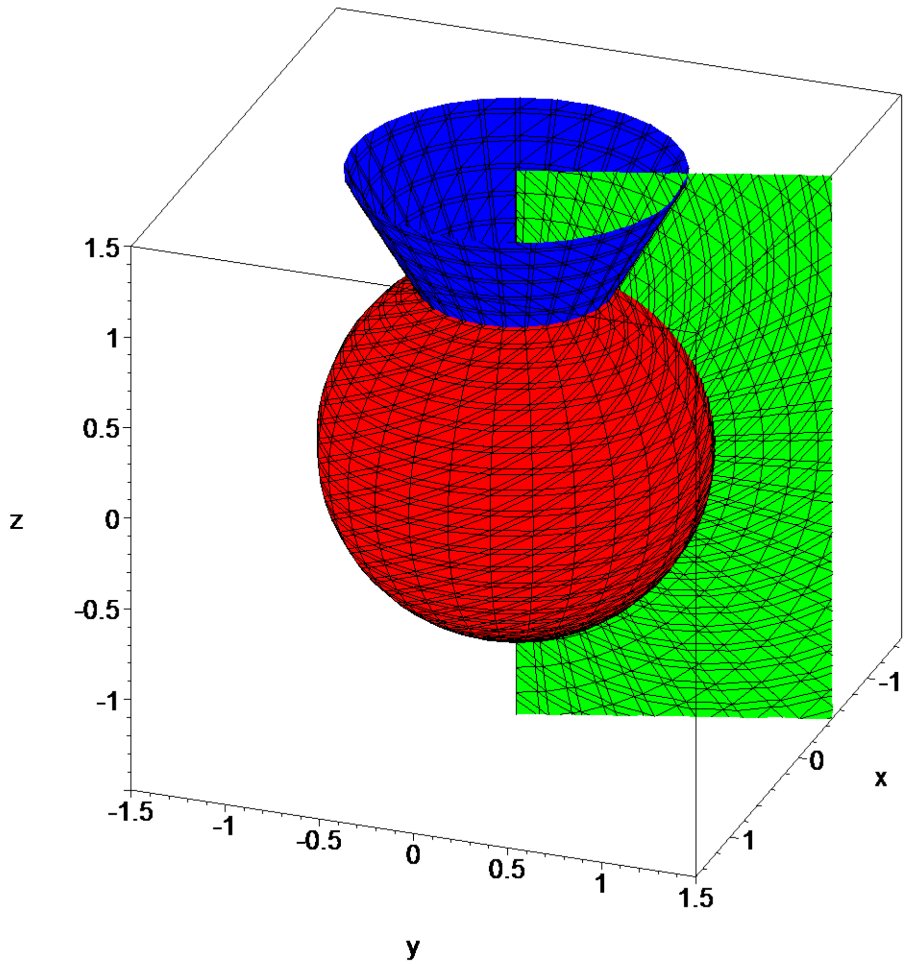
- angular-momentum quantum number j, which is invariably positive and assumes only two values based on l, specifically $j = l + \frac{1}{2}$ or $j = l - \frac{1}{2}$, and

- magnetic quantum number m, which assumes all half-integer values from $-j$ to $+j$, and which is hence better designated as m_j to distinguish it from m_l that arises from Schroedinger's equation, cf. section 12b53. The coefficient of $i\,\phi$ in exponential term in a solution of Dirac's equation is $m_j + \frac{1}{2}$ or $m_j - \frac{1}{2}$, i.e. an integer, so that the condition of periodicity is fulfilled, so $\mathbf{e}^{\left(i\left(m_j + \frac{1}{2}\right)\phi\right)}$ or $\mathbf{e}^{\left(i\left(m_j - \frac{1}{2}\right)\phi\right)}$. To avoid complications of notation we use simply m instead of m_j in the following treatment.

Unlike the solutions of Schroedinger's temporally independent equation that one represents as $\psi_{k,\,l,\,m}(r, \theta, \phi)$ in spherical polar coordinates with quantum numbers k, l, m for which in general a particular amplitude function is not associated with a specific state of the hydrogen atom as defined with its energy and angular momentum, for these solutions of the Dirac equation each amplitude function is associated with a particular spectrometric state specified with those four quantum numbers . In spherical polar coordinates r, θ, ϕ, as defined in this plot, with a sphere for distance coordinate r, a cone about the polar axis for angular coordinate θ and a half-plane for angular coordinate ϕ,

```
> addcoords(scispherical,[r,theta,phi],[r*sin(theta)*cos(phi),r*s
  in(theta)*sin(phi),r*cos(theta)]);
> plots[implicitplot3d]([r=1, theta=Pi/6, phi=3*Pi/5], r=0..4,
  theta=0..Pi, phi=0..2*Pi,
            axes=boxed,  colour=[red, blue, green],
  titlefont=[TIMES,BOLD,14], labels=["x","y","z"],
            grid=[30,30,30], view=[-1.5..1.5,-1.5..1.5,
  -1.5..1.5], scaling=constrained,
            title="surfaces of r=1 red, theta=Pi/6 blue,
  phi=3*Pi/5 green",
            coords=scispherical, orientation=[20,65]);
```

surfaces of r=1 red, theta=Pi/6 blue, phi=3*Pi/5 green



>

we present, in terms of these quantum numbers in Dirac notation as kets of form |*n*, *l*, *j*, *m*>, in vectorial form several eigenfunctions of an atom of atomic number *Z* with one electron assuming distances in terms of $\frac{a_0}{Z}$, in which appear Bohr radius a_0 and proton number *Z*, and eigenfunctions in terms of $\sqrt{\frac{Z^3}{\pi\, a_0^{\,3}}}$, as specified above; α that appears in these expressions denotes the dimensionless physical parameter known as the fine-structure constant, $\alpha = \frac{e^2}{2\, \varepsilon_0\, h\, c}$ = 0.0072973525664 ~1/137, and has no relation to the Dirac matrices above. Rather than to derive the solutions to Dirac's equation as amplitude functions, we present these approximate formulae, which lack normalising factors and which include terms of order only αZ, that appear in a paper by R. E. Powell (*Journal of Chemical Education*, 45 (9), 558 - 563, 1968). The name of each formula is precisely a ket function | > of which the four arugments are identically the four quantum numbers; the amplitude function hence precisely identies uniquely the state of the atom with one electron.

```
> `|1,0,1/2,1/2>` :=
  <exp(-r),0,1/2*I*alpha*Z*exp(-r)*cos(theta),1/2*I
                              *alpha*Z*exp(-r)*sin(theta)*exp(I*phi)>;
```

$$|1,0,1/2,1/2> := \begin{bmatrix} \mathbf{e}^{(-r)} \\ 0 \\ \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \cos(\theta) \\ \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \sin(\theta) \mathbf{e}^{(\phi I)} \end{bmatrix}$$

```
> `|1,0,1/2,-1/2>` :=
  <0,-exp(-r),-1/2*I*alpha*Z*exp(-r)*sin(theta)

  *exp(-I*phi),1/2*I*alpha*Z*exp(-r)*cos(theta)>;
```

$$|1,0,1/2,\text{-}1/2> := \begin{bmatrix} 0 \\ -\mathbf{e}^{(-r)} \\ \frac{-1}{2} I \alpha Z \mathbf{e}^{(-r)} \sin(\theta) \mathbf{e}^{(-I\phi)} \\ \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \cos(\theta) \end{bmatrix}$$

```
> `|2,0,1/2,1/2>` :=
  sqrt(1/8)*<(1-r/2)*exp(-r/2),0,1/2*I*alpha*Z*(1-r/4)*exp(-r/2)

  *cos(theta),1/2*I*alpha*Z*(1-r/4)*exp(-r/2)*sin(theta)*exp(I*ph
  i)>;
```

$$|2,0,1/2,1/2> := \begin{bmatrix} \frac{1}{4}\sqrt{2}\left(1-\frac{r}{2}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)} \\ 0 \\ \frac{1}{8} I \sqrt{2}\, \alpha Z \left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)} \cos(\theta) \\ \frac{1}{8} I \sqrt{2}\, \alpha Z \left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\, \mathbf{e}^{(\phi I)} \end{bmatrix}$$

```
> `|2,0,1/2,-1/2>` :=
  sqrt(1/8)*<0,-(1-r/2)*exp(-r/2),-1/2*I*alpha*Z*(1-r/4)*exp(-r/2
```

```
)

*sin(theta)*exp(-I*phi),1/2*I*alpha*Z*(1-r/4)*exp(-r/2)*cos(the
ta)>;
```

$$|2,0,1/2,-1/2> := \begin{bmatrix} 0 \\ -\frac{1}{4}\sqrt{2}\left(1-\frac{r}{2}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)} \\ \frac{-1}{8} I\sqrt{2}\,\alpha Z\left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\,\mathbf{e}^{(-I\,\phi)} \\ \frac{1}{8} I\sqrt{2}\,\alpha Z\left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)}\cos(\theta) \end{bmatrix}$$

```
> `|2,1,1/2,1/2>` :=
sqrt(1/32)*<-sqrt(1/3)*r*exp(-r/2)*cos(theta),-sqrt(1/3)*r*exp(
-r/2)

*sin(theta)*exp(I*phi),sqrt(3/4)*I*alpha*Z*(1-r/6)*exp(-r/2),0>
;
```

$$|2,1,1/2,1/2> := \begin{bmatrix} -\frac{1}{24}\sqrt{2}\sqrt{3}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\cos(\theta) \\ -\frac{1}{24}\sqrt{2}\sqrt{3}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\,\mathbf{e}^{(\phi\,I)} \\ \frac{1}{16} I\sqrt{2}\sqrt{3}\,\alpha Z\left(1-\frac{r}{6}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)} \\ 0 \end{bmatrix}$$

```
> `|2,1,1/2,-1/2>` :=
sqrt(1/32)*<sqrt(1/3)*r*exp(-r/2)*sin(theta)*exp(-I*phi),-sqrt(
1/3)

*r*exp(-r/2)*cos(theta),0,sqrt(3/4)*I*alpha*Z*(1-r/6)*exp(-r/2)
>;
```

$$|2,1,1/2,-1/2> := \begin{bmatrix} \frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\, \mathbf{e}^{(-I\,\phi)} \\ -\frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \cos(\theta) \\ 0 \\ \frac{1}{16} I \sqrt{2}\sqrt{3}\, \alpha\, Z \left(1-\frac{r}{6}\right) \mathbf{e}^{\left(-\frac{r}{2}\right)} \end{bmatrix}$$

```
> `|2,1,3/2,3/2>` :=
  sqrt(1/32)*<sqrt(1/2)*r*exp(-r/2)*sin(theta)*exp(I*phi),0,sqrt(
  1/32)

  *I*alpha*Z*r*exp(-r/2)*sin(theta)*cos(theta)*exp(I*phi),

  sqrt(1/32)*I*alpha*Z*r*exp(-r/2)*sin(theta)^2*exp(2*I*phi)>;
```

$$|2,1,3/2,3/2> := \begin{bmatrix} \frac{1}{8} r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\, \mathbf{e}^{(\phi\, I)} \\ 0 \\ \frac{1}{32} I\, \alpha\, Z\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\, \mathbf{e}^{(\phi\, I)} \\ \frac{1}{32} I\, \alpha\, Z\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2\, \mathbf{e}^{(2\, I\, \phi)} \end{bmatrix}$$

```
> `|2,1,3/2,-3/2>` :=
  sqrt(1/32)*<0,sqrt(1/2)*r*exp(-r/2)*sin(theta)*exp(-I*phi),sqrt
  (1/32)

  *I*alpha*Z*r*exp(-r/2)*sin(theta)^2*exp(-2*I*phi),

  -sqrt(1/32)*I*alpha*Z*r*exp(-r/2)*sin(theta)*cos(theta)*exp(-I*
  phi)>;
```

$$|2,1,3/2,-3/2> := \begin{bmatrix} 0 \\ \frac{1}{8} r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\, \mathbf{e}^{(-I\,\phi)} \\ \frac{1}{32} I\, \alpha\, Z\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2\, \mathbf{e}^{(-2\, I\, \phi)} \\ \frac{-1}{32} I\, \alpha\, Z\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\, \mathbf{e}^{(-I\,\phi)} \end{bmatrix}$$

```
> `|2,1,3/2,1/2>` :=
sqrt(1/32)*<sqrt(2/3)*r*exp(-r/2)*cos(theta),-sqrt(1/6)*r*exp(-r/2)
*sin(theta)*exp(I*phi),sqrt(3/32)*I*alpha*Z*r*exp(-r/2)*(cos(theta)^2-1/2),
sqrt(3/32)*I*alpha*Z*r*exp(-r/2)*sin(theta)*cos(theta)*exp(I*phi)>;
```

$$|2,1,3/2,1/2> := \begin{bmatrix} \frac{1}{24}\sqrt{2}\sqrt{6}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\cos(\theta) \\ -\frac{1}{48}\sqrt{2}\sqrt{6}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\,\mathbf{e}^{(\phi I)} \\ \frac{1}{64}I\sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\left(\cos(\theta)^2-\frac{1}{2}\right) \\ \frac{1}{64}I\sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\,\mathbf{e}^{(\phi I)} \end{bmatrix}$$

```
> `|2,1,3/2,-1/2>` :=
sqrt(1/32)*<-sqrt(1/6)*r*exp(-r/2)*sin(theta)*exp(-I*phi),-sqrt(2/3)*r*exp(-r/2)
*cos(theta),-sqrt(3/32)*I*alpha*Z*r*exp(-r/2)*sin(theta)*cos(theta)
*exp(-I*phi),sqrt(3/32)*I*alpha*Z*r*exp(-r/2)*(cos(theta)^2-1/2)>;
```

$$|2,1,3/2,-1/2> := \begin{bmatrix} -\frac{1}{48}\sqrt{2}\sqrt{6}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\,\mathbf{e}^{(-I\phi)} \\ -\frac{1}{24}\sqrt{2}\sqrt{6}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\cos(\theta) \\ \frac{-1}{64}I\sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\,\mathbf{e}^{(-I\phi)} \\ \frac{1}{64}I\sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\left(\cos(\theta)^2-\frac{1}{2}\right) \end{bmatrix}$$

The notable characteristics of these vectorial amplitude functions follow:

- of the four components of the vectors, one of which might be zero, two, specifically ψ_3 and ψ_4, contain, if not zero, product αZ that, for $Z < 10$, produces magnitudes of these components much smaller than components ψ_1 and ψ_2 if not zero;

- we thus describe ψ_1 and ψ_2 as the large components and ψ_3 and ψ_4 as the small components;
- each component of the four might in general be complex, having both real and imaginary parts; there are hence up to eight distinguishable parts of a particular vectorial amplitude function, and
- the square $\psi^* \psi$ of each amplitude function has only real parts, both small that contain $\alpha^2 Z^2$ and large, as calculations below demonstrate.

The energies associated with these amplitude functions are expressible as, with $Z2 = Z^2$ before the Taylor expansion below,

```
> E[n,j] := m[e]*c^2/sqrt(1 + Z2*alpha^2/(k +
  sqrt((j+1/2)^2+Z2*alpha^2))^2);
```

$$E_{n,j} := \frac{m_e c^2}{\sqrt{1 + \frac{Z2\,\alpha^2}{\left(k + \frac{\sqrt{4\,Z2\,\alpha^2 + 4\,j^2 + 4\,j + 1}}{2}\right)^2}}}$$

in which k is a quantum number analogous to radial quantum number k in the solution of Schroedinger's equation for the hydrogen atom in spherical polar coordinates as the number of radial nodes. Here, $k = n - \left(j + \frac{1}{2}\right)$, which we insert.

```
> E[n,j] := subs(k=n-(j+1/2), E[n,j]);
```

$$E_{n,j} := \frac{m_e c^2}{\sqrt{1 + \frac{Z2\,\alpha^2}{\left(n - j - \frac{1}{2} + \frac{\sqrt{4\,Z2\,\alpha^2 + 4\,j^2 + 4\,j + 1}}{2}\right)^2}}}$$

When we make a Taylor expansion in $Z2$ and replace that with Z^2,

```
> E[n,j] := subs(Z2=Z^2, taylor(E[n,j], Z2, 3)) assuming
  positive;
```

$$E_{n,j} := m_e c^2 - \frac{1}{2}\frac{m_e c^2 \alpha^2}{n^2} Z^2 + m_e c^2 \left(\frac{\alpha^4}{n^3 (1 + 2\,j)} + \frac{3\,\alpha^4}{8\,n^4}\right) Z^4 + \mathrm{O}(Z^6)$$

we find that the first term in the result is just the energy associated with the rest mass of the electron, the second term is equal to the energy of the hydrogen atom with $Z = 1$ as deduced by Balmer and Rydberg from experiment and as reproduced in the derivation with Schroedinger's equations, and the third and further terms are relativistic corrections to the energy that produce the splitting of the otherwise degenerate energies of states with common n, as discussed in section 12b.53.

We proceed to plot some amplitude functions among those listed above. As we cannot plot an eigenfunction directly because it comprises a vector of four components, we plot successively in spherical polar coordinates the separate components in their real and imaginary parts and then the squared amplitude function $|\psi^2| = \psi^* \psi$, in which ψ^* implies the complex conjugate of ψ, in its large and small parts. The lack of normalising factor has no effect on the shape of the plotted objects because we select a value of ψ that is $\frac{1}{100}$ of its maximum value; the resulting surface hence would contain 0.995 of the total density of electronic charge, consistent with plots of amplitude functions from the solutions of the Schroedinger equation in other sections.

```
> cond := [Z=1, alpha=0.0072973525664];
```

$$cond := [Z = 1, \alpha = 0.0072973525664]$$

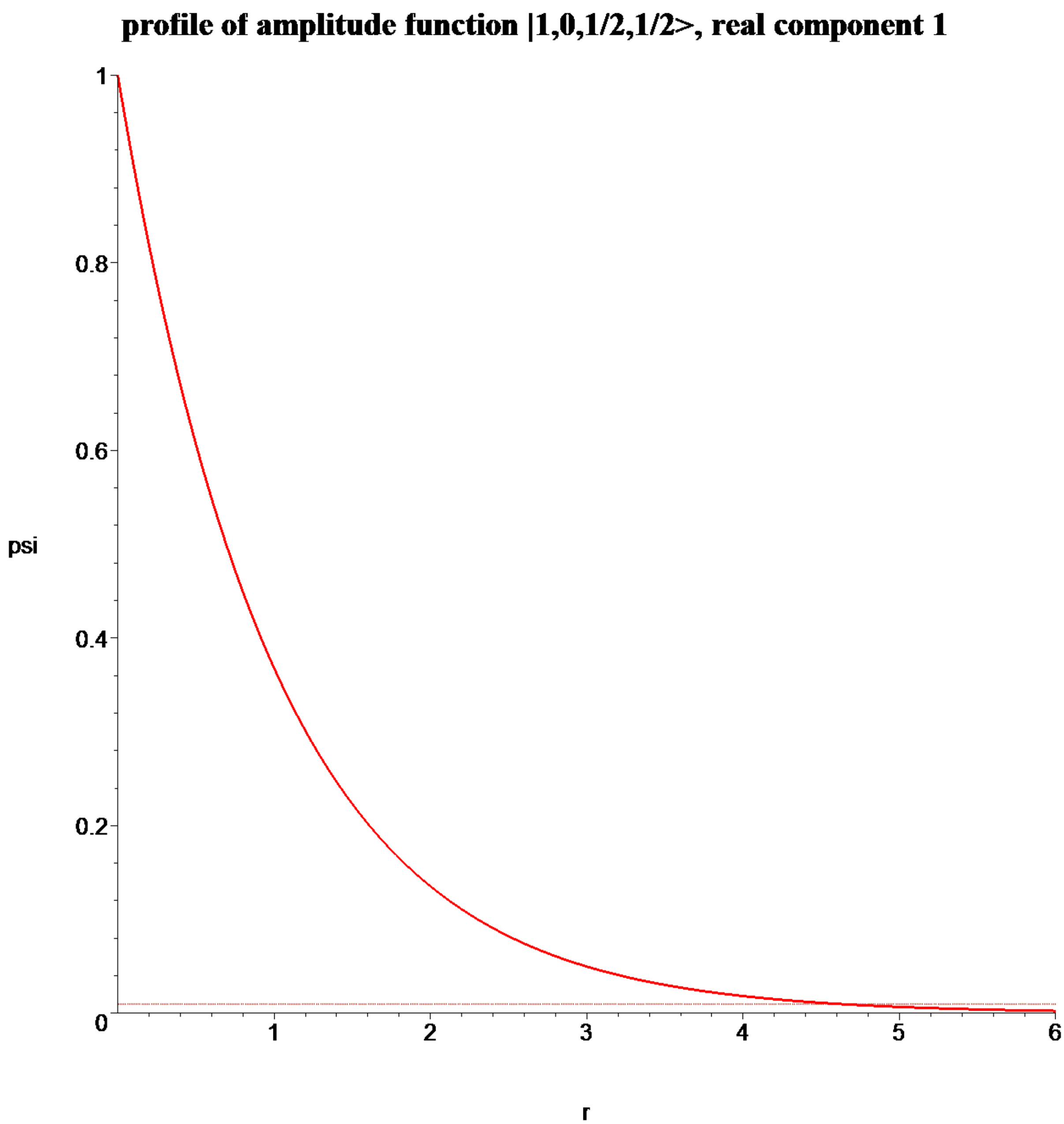
We recall first |1,0,1/2,1/2> as a vector with four components in an unnormalised form,

```
> '`|1,0,1/2,1/2>`' = `|1,0,1/2,1/2>`;
```

$$|1,0,1/2,1/2> = \begin{bmatrix} \mathbf{e}^{(-r)} \\ 0 \\ \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \cos(\theta) \\ \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \sin(\theta) \mathbf{e}^{(\phi I)} \end{bmatrix}$$

and plot the radial profile of the first component of |1,0,1/2,1/2>.

```
> plot([`|1,0,1/2,1/2>`[1], 0.01], r=0..6, 0..1, title=
    "profile of amplitude function |1,0,1/2,1/2>, real component
  1",
    titlefont=[TIMES,BOLD,14], colour=[red, brown],
  linestyle=[1,2],
    labels=["r", "psi"], thickness=[3,2]);
```



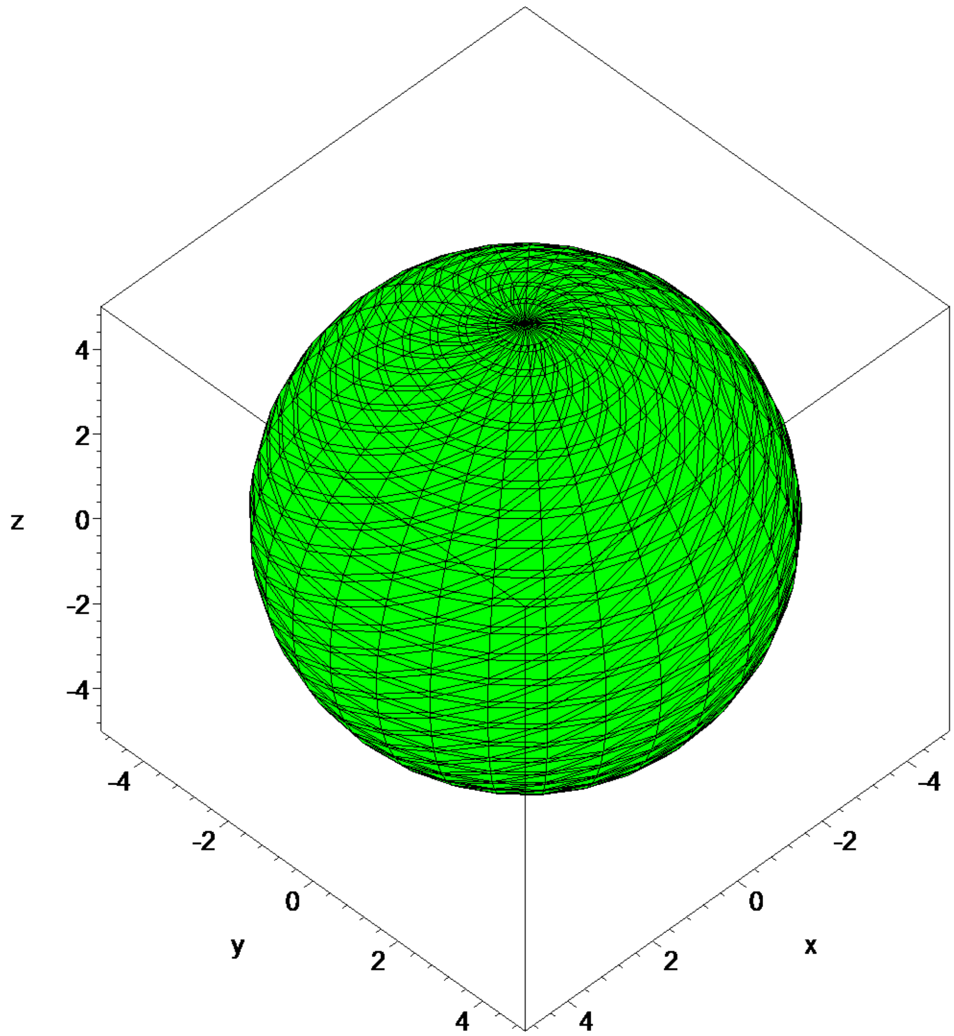

```
>
```

We plot the surface of this first component of |1,0,1/2,1/2>

```
> plots[implicitplot3d](`|1,0,1/2,1/2>`[1]=0.01,
     r=0..5, theta=0..Pi, phi=0..2*Pi, colour=green,
  labels=["x","y","z"],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |1,0,1/2,1/2>, real component 1",

     titlefont=[TIMES,BOLD,14], view=[-5..5,-5..5,-5..5]);
```

amplitude function |1,0,1/2,1/2>, real component 1




```
>
```

which generates a perfect sphere because this component has no angular dependence. Whereas the second component is identically zero, the third component is purely imaginary;

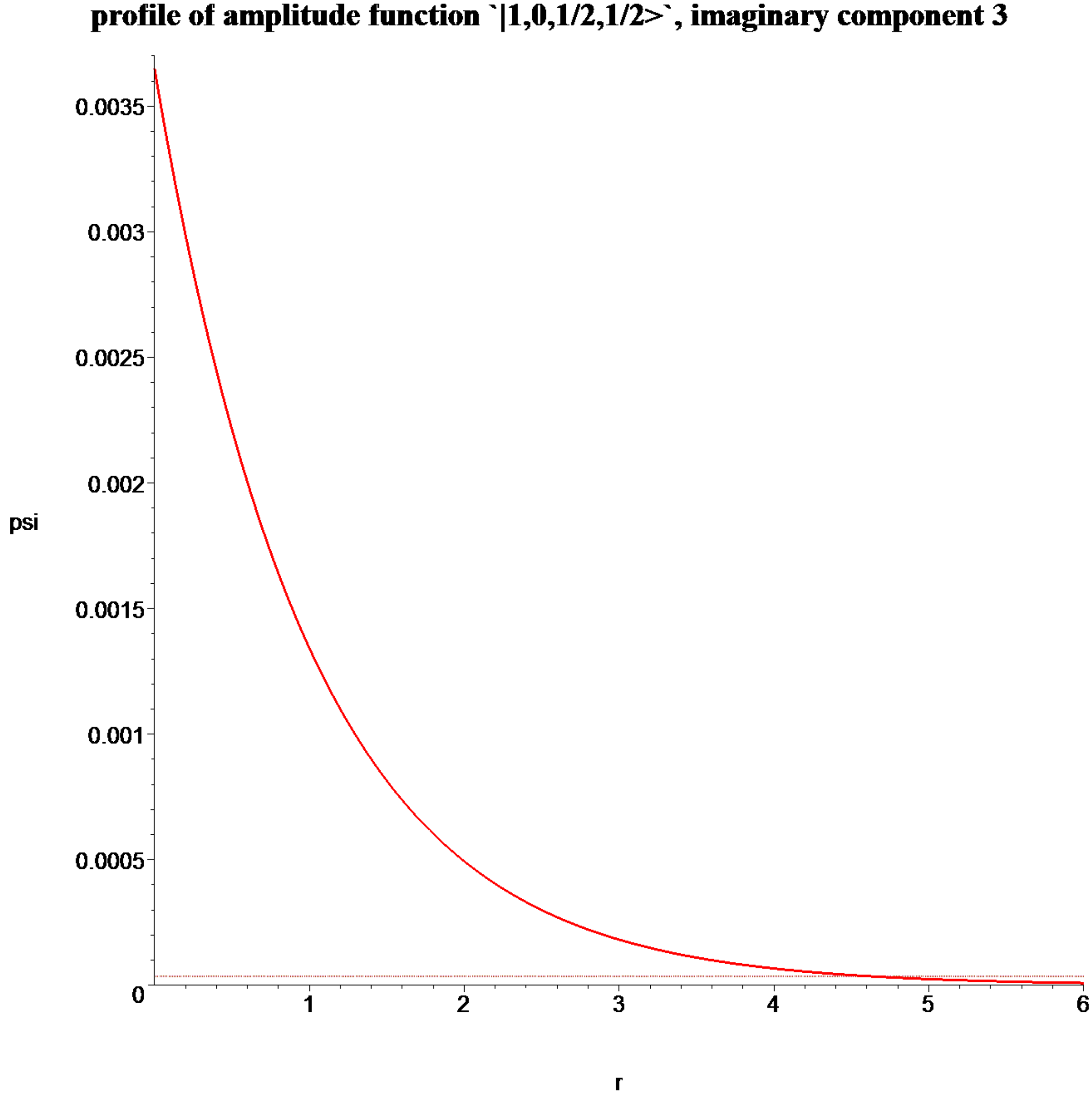
```
> '`|1,0,1/2,1/2>`'[3] = `|1,0,1/2,1/2>`[3];
```

$$|1,0,1/2,1/2\rangle_3 = \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \cos(\theta)$$

we plot first the radial profile along the polar axis, for which $\theta = 0$, to obtain the criterion for the surface,

```
> plot([eval(Im(`|1,0,1/2,1/2>`[3]), [theta=0,op(cond)]),
  0.0000365], r=0..6, 0..0.0037,
     title="profile of amplitude function `|1,0,1/2,1/2>`,
  imaginary component 3",
```

```
   titlefont=[TIMES,BOLD,14], colour=[red, brown],
linestyle=[1,2],
   labels=["r", "psi"], thickness=[3,2]);
```



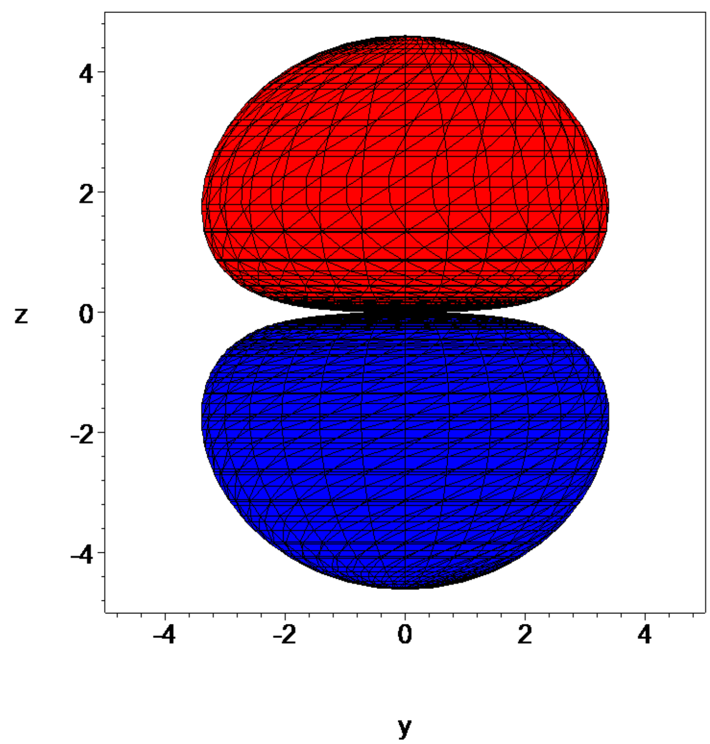
>

in which the maximum amplitude is 0.00365, much less than unity for the first component, and then the surface itself.

```
> plots[implicitplot3d]([eval(Im(`|1,0,1/2,1/2>`[3]),
cond)=0.0000365,
   eval(Im(`|1,0,1/2,1/2>`[3]), cond)=-0.0000365], r=0..5,
theta=0..Pi,
   phi=0..2*Pi, colour=[red, blue], orientation=[0,90],
labels=["x","y","z"],
```

```
   coords = scispherical, grid=[30,30,30], scaling=constrained,
axes=box,
   title="amplitude function |1,0,1/2,1/2>, imaginary component
3",
   titlefont=[TIMES,BOLD,14], view=[-5..5,-5..5,-5..5]);
```

amplitude function |1,0,1/2,1/2>, imaginary component 3




```
>
```

The fourth component,

```
> '`|1,0,1/2,1/2>`'[4] = evalc(`|1,0,1/2,1/2>`[4]);
```

$$|1,0,1/2,1/2>_4 = -\frac{1}{2}\alpha Z \mathbf{e}^{(-r)} \sin(\theta)\sin(\phi) + \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \sin(\theta)\cos(\phi)$$

has both real and imaginary parts, of which we select those parts separately.

```
> rp := Re(rhs(%)) assuming real;
```

$$rp := -\frac{1}{2}\,\alpha\,Z\,\mathbf{e}^{(-r)}\,\sin(\theta)\,\sin(\phi)$$

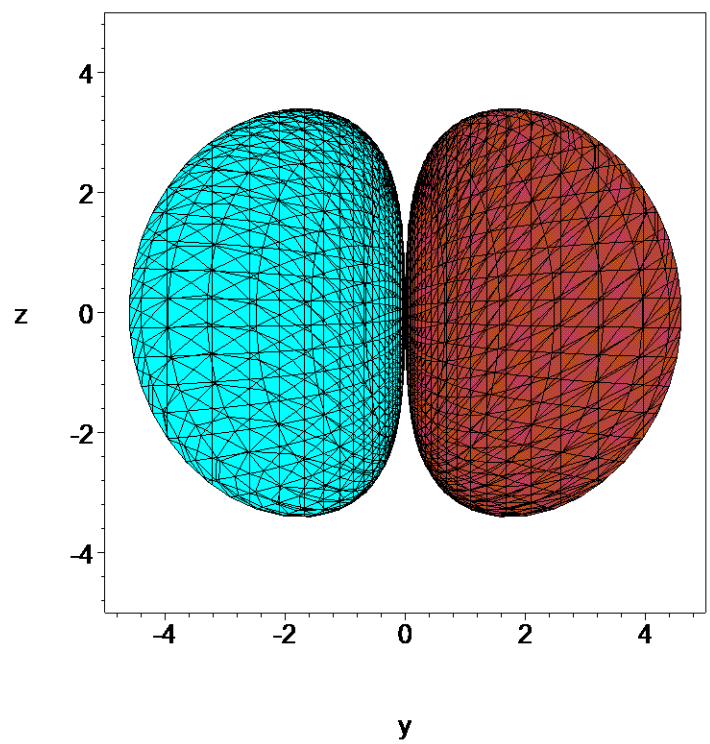
```
> ip := Im(rhs(%%)) assuming real;
```

$$ip := \frac{1}{2}\,\alpha\,Z\,\mathbf{e}^{(-r)}\,\sin(\theta)\,\cos(\phi)$$

We plot the surface itself in its real,

```
> plots[implicitplot3d]([eval(rp, cond)=0.0000365,
     eval(rp, cond)=-0.0000365], r=0..5, theta=0..Pi,
  phi=0..2*Pi,
     labels=["x","y","z"], colour=[cyan, brown],
  orientation=[0,90],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |1,0,1/2,1/2>, component 4, real
  part",
     titlefont=[TIMES,BOLD,14], view=[-5..5,-5..5,-5..5]);
```

amplitude function |1,0,1/2,1/2>, component 4, real part

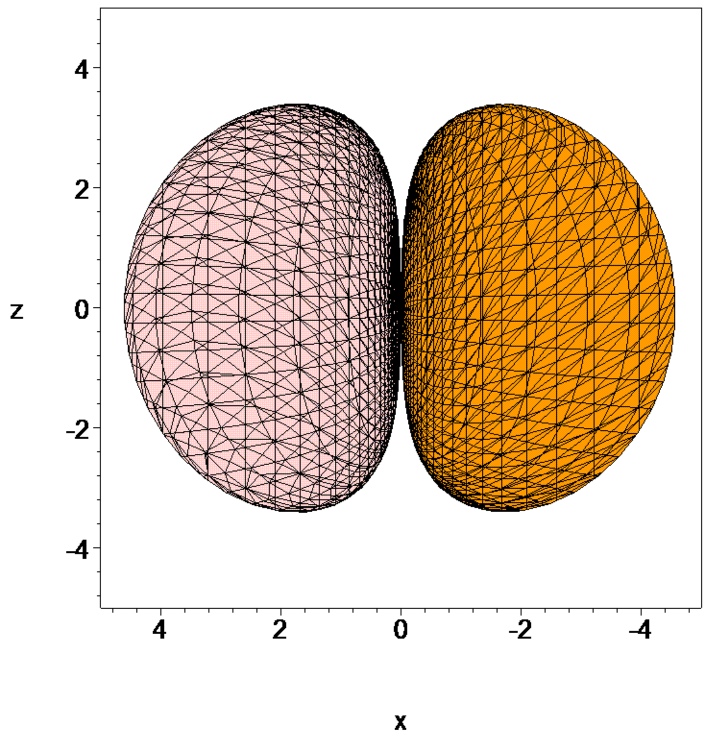



```
>
```

and imaginary parts.

```
> plots[implicitplot3d]([eval(ip, cond)=0.0000365,
    eval(ip, cond)=-0.0000365], r=0..5, theta=0..Pi,
  phi=0..2*Pi,
    colour=[pink, coral], orientation=[90,90],
  labels=["x","y","z"],
    coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
    title="amplitude function |1,0,1/2,1/2>, component 4,
  imaginary part",
    titlefont=[TIMES,BOLD,14], view=[-5..5,-5..5,-5..5]);
```

amplitude function |1,0,1/2,1/2>, component 4, imaginary part



\>

The surfaces in the preceding three plots resemble perfectly the surfaces of the amplitude functions $\psi_{0,\,1,\,0}(r, \theta, \phi)$ and the real and imaginary parts of $\psi_{0,\,1,\,1}(r, \theta, \phi)$. From |1,0,1/2,1/2>,

```
> p := evalc(`|1,0,1/2,1/2>`);
```

$$p := \begin{bmatrix} \mathbf{e}^{(-r)} \\ 0 \\ \frac{1}{2} I\, \alpha\, Z\, \mathbf{e}^{(-r)} \cos(\theta) \\ -\frac{1}{2} \alpha\, Z\, \mathbf{e}^{(-r)} \sin(\theta) \sin(\phi) + \frac{1}{2} I\, \alpha\, Z\, \mathbf{e}^{(-r)} \sin(\theta) \cos(\phi) \end{bmatrix}$$

and its complex conjugate,

```
> pc := evalc(subs(I=-I,`|1,0,1/2,1/2>`));
```

$$pc := \begin{bmatrix} \mathbf{e}^{(-r)} \\ 0 \\ \frac{-1}{2} I\,\alpha\,Z\,\mathbf{e}^{(-r)}\cos(\theta) \\ -\frac{1}{2}\alpha\,Z\,\mathbf{e}^{(-r)}\sin(\theta)\sin(\phi) - \frac{1}{2} I\,\alpha\,Z\,\mathbf{e}^{(-r)}\sin(\theta)\cos(\phi) \end{bmatrix}$$

we form scalar product |1,0,1/2,1/2>* **.** |1,0,1/2,1/2>,

```
> ps :=
  simplify(evalc(expand(subs(I=-I,LinearAlgebra:-Transpose(`|1,0,
  1/2,1/2>`)) . `|1,0,1/2,1/2>`))) assuming real;
```

$$ps := \frac{1}{4}\mathbf{e}^{(-2\,r)}\,(Z^2\,\alpha^2 + 4)$$

which is entirely real and which we separate into two parts -- large that does not contain α and small that contains α. This formula lacks the normalising factor from |1,0,1/2,1/2>, which would result in multiplicand $\frac{Z^3}{\pi\,a_0^{\,3}}$ in the total expression above for the scalar product.

```
> fl := simplify(remove(has, expand(ps), alpha));
```

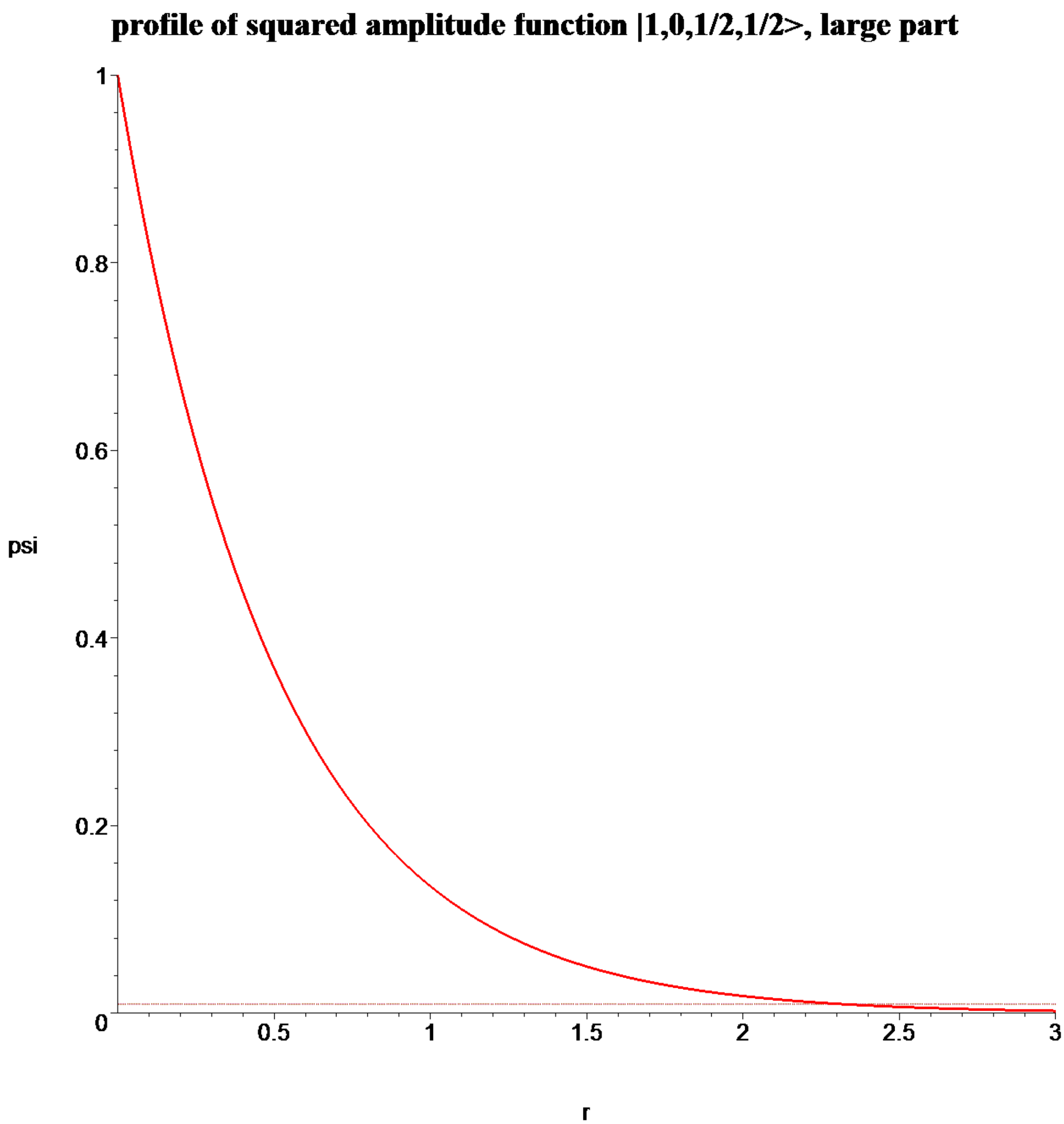
$$fl := \mathbf{e}^{(-2\,r)}$$

```
> fs := simplify(ps - fl);
```

$$fs := \frac{1}{4}\mathbf{e}^{(-2\,r)}\,Z^2\,\alpha^2$$

We plot the radial profile of its large part,

```
> plot([eval(fl, cond), 0.01], r=0..3, 0..1, labels=["r", "psi"],
  thickness=[3,2],
     linestyle=[1,2], titlefont=[TIMES,BOLD,14], colour=[red,
  brown],
     title="profile of squared amplitude function |1,0,1/2,1/2>,
  large part");
```

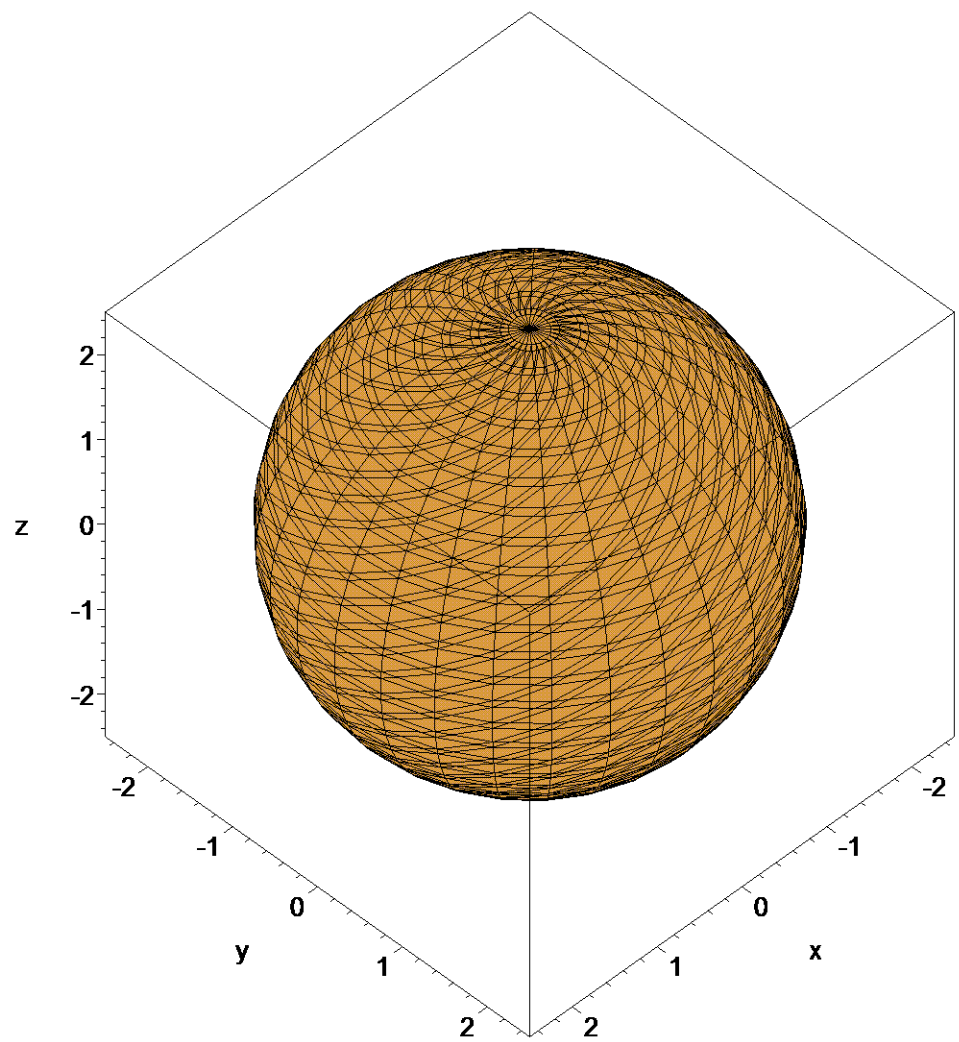



```
>
```

and the surface of that squared |1,0,1/2,1/2> .

```
> plots[implicitplot3d](eval(fl, cond)=0.01, r=0..3, theta=0..Pi,
    phi=0..2*Pi, colour=gold, orientation=[45,45],
  labels=["x","y","z"],
    coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
    title="squared amplitude function |1,0,1/2,1/2>, large
  part",
    titlefont=[TIMES,BOLD,14],
  view=[-2.5..2.5,-2.5..2.5,-2.5..2.5]);
```

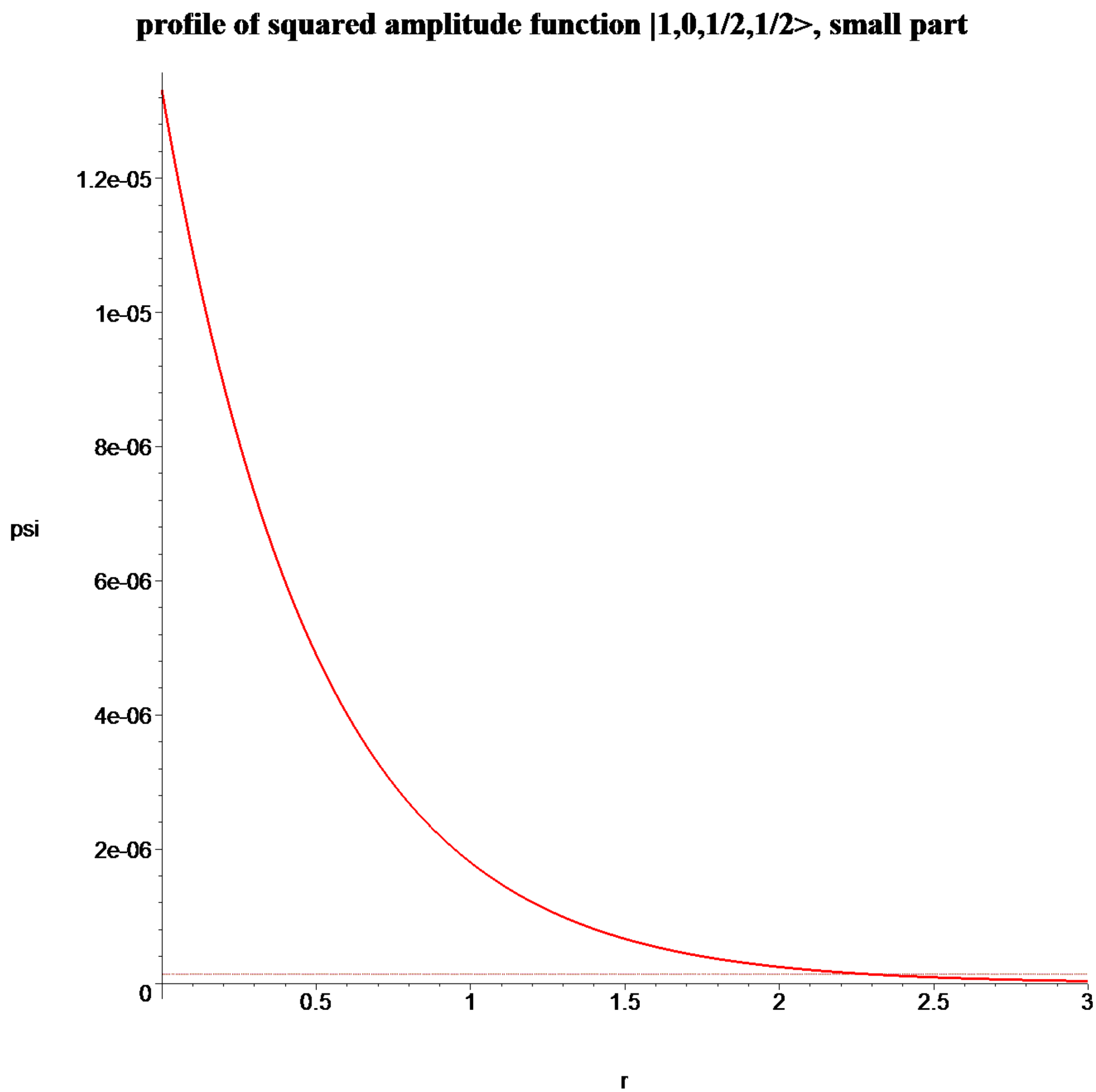
squared amplitude function |1,0,1/2,1/2>, large part




```
>
```

The small part comprises one term, specified above,

```
> plot([eval(fs, cond), 1.33e-7], r=0..3, labels=["r", "psi"],
  thickness=[3,2],
     linestyle=[1,2], titlefont=[TIMES,BOLD,14], colour=[red,
  brown],
     title="profile of squared amplitude function |1,0,1/2,1/2>,
  small part");
```

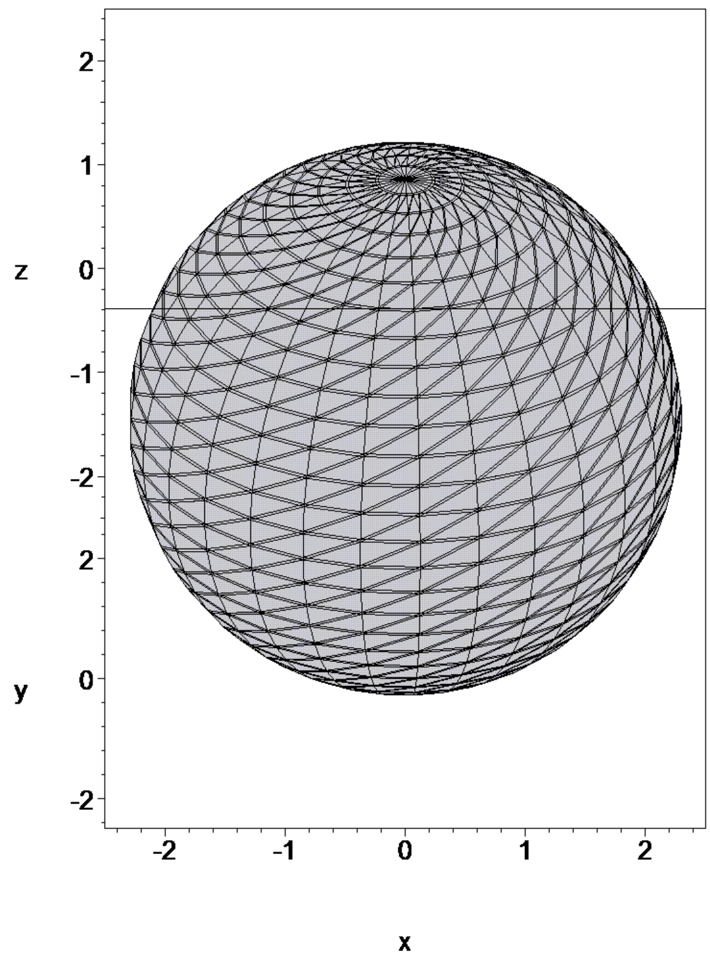


>

of which we accordingly plot the surface of the small part of |1,0,1/2,1/2> squared containing α,

```
> plots[implicitplot3d](eval(fs, cond)=1.33e-7, r=0..3.5,
  theta=0..Pi, phi=0..2*Pi,
     colour=grey, orientation=[-90,60],coords = scispherical,
  grid=[30,30,30],
     scaling=constrained, axes=box,
  view=[-2.5..2.5,-2.5..2.5,-2.5..2.5],
     title="squared amplitude function |1,0,1/2,1/2>, small
  part",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14]);
```

squared amplitude function |1,0,1/2,1/2>, small part



>

which is again a perfect sphere; the surfaces of both large and small parts hence plot as spheres that have the same diameter and are hence indistinguishable; if the criterion of the small term were not $\frac{1}{100}$ times its maximum amplitude but $\frac{1}{100}$ times the maximum amplitude of the large part, the surface of the small part would be insignificant for $Z = 1$, and analogously for the small parts of succeeding squares of amplitude functions.

According to these plots of profiles and surfaces of amplitude function |1,0,1/2,1/2> for the hydrogen atom in its state of least energy as derived from Dirac's equation, of the four components the spherically symmetric characteristic of the first component is similar to that of $\psi_{0,\,0,\,0}$ from Schroedinger's temporally independent equation that yields $\psi_{k,\,l,\,m}$, but there are two further components not zero that might have both real and imaginary parts; their surfaces are not spherically symmetric but cylindrically symmetric about the polar axis for the real third component, similar to $\psi_{0,\,1,\,0}$ from Schroedinger's equation, and cylindrically symmetric equivalent to $\psi_{0,\,1,\,0}$ rotated about the other two cartesian axes for the real and imaginary parts of the fourth part. The maximum amplitudes of the third and fourth components are much smaller than the maximum amplitude of the first component because of factor $\alpha^2 Z^2$, which for $Z = 1$ of hydrogen evaluates to $\alpha^2 Z^2 = 5.325\ 10^{(-5)}$; for an atomic nucleus of large atomic number the third and fourth components would have much larger relative maximum amplitudes. For this squared amplitude function |1,0,1/2,1/2> that is entirely real, both terms yield spherical surfaces. The squared amplitude function, $|\psi^2| = \psi^* \psi$, must contain only real parts; the density of electronic charge in the vicinity of the atomic nucleus is supposed to be proportional to this squared quantity as a probability density. Dirac's two coupled differential equations of first order for the large part hence produce results similar to Schroedinger's single differential equation of second order.

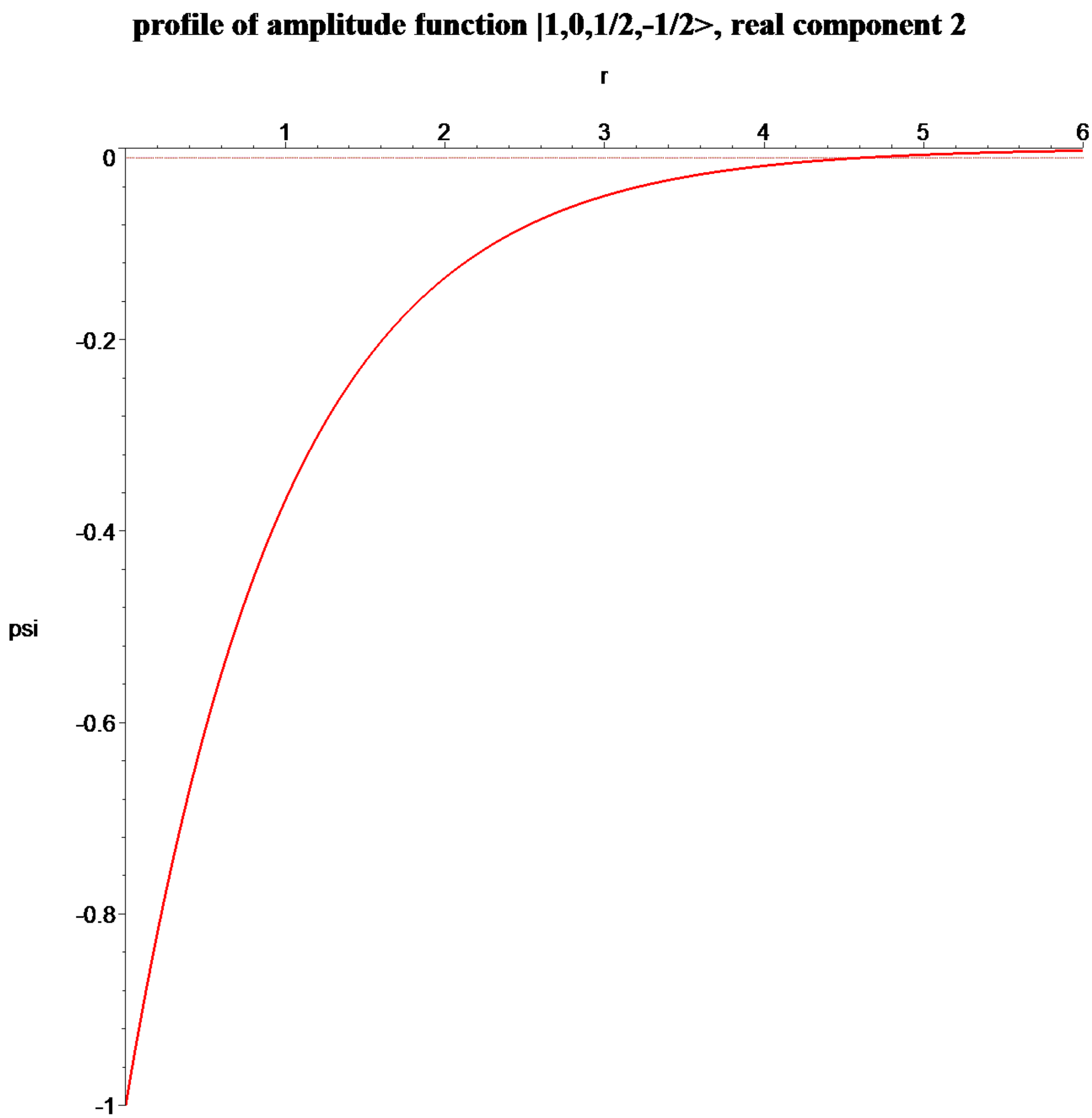
We proceed to recall |1,0,1/2,-1/2> .

```
> '`|1,0,1/2,-1/2>`' = `|1,0,1/2,-1/2>`;
```

$$|1,0,1/2,-1/2> = \begin{bmatrix} 0 \\ -\mathbf{e}^{(-r)} \\ \frac{-1}{2} I\,\alpha\,Z\,\mathbf{e}^{(-r)} \sin(\theta)\,\mathbf{e}^{(-I\,\phi)} \\ \frac{1}{2} I\,\alpha\,Z\,\mathbf{e}^{(-r)} \cos(\theta) \end{bmatrix}$$

As the first component of |1,0,1/2,-1/2> is zero, we plot the radial profile of the second component.

```
> plot([`|1,0,1/2,-1/2>`[2], -0.01], r=0..6, -1..0,
    title="profile of amplitude function |1,0,1/2,-1/2>, real
  component 2",
    titlefont=[TIMES,BOLD,14], colour=[red, brown],
  linestyle=[1,2],
    labels=["r", "psi"], thickness=[3,2]);
```



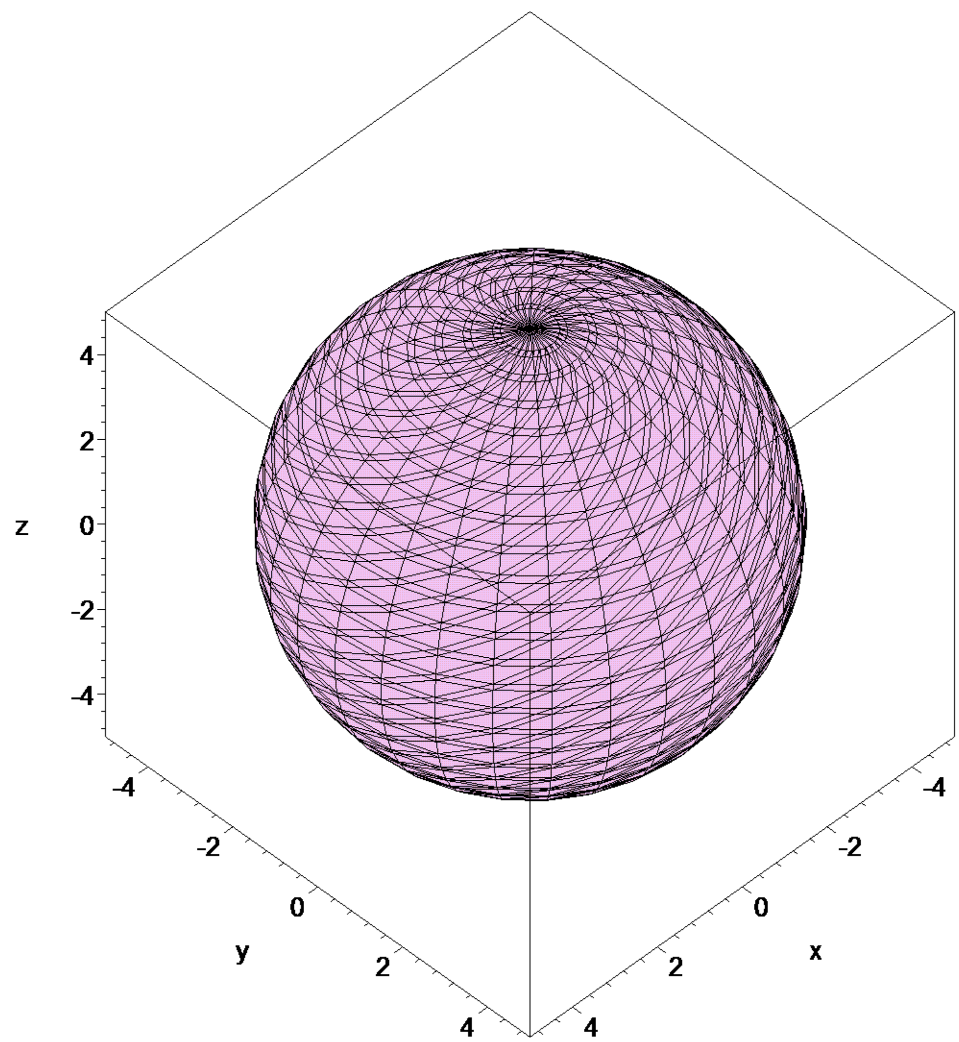

```
>
```

We plot the surface of this negative second component of |1,0,1/2,-1/2> at a value of ψ that is $\frac{1}{100}$ of its maximum magnitude,

```
> plots[implicitplot3d](`|1,0,1/2,-1/2>`[2]=-0.01,
    r=0..5, theta=0..Pi, phi=0..2*Pi, colour=plum,
  labels=["x","y","z"],
    coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
    title="amplitude function |1,0,1/2,-1/2>, real component 2",

    titlefont=[TIMES,BOLD,14], view=[-5..5,-5..5,-5..5]);
```

amplitude function |1,0,1/2,-1/2>, real component 2



>

which generates a perfect sphere because this component has no angular dependence. The third component has both real and imaginary parts,

```
> '`|1,0,1/2,-1/2>`'[3] = evalc(`|1,0,1/2,-1/2>`[3]);
```

$$|1,0,1/2,-1/2>_3 = -\frac{1}{2}\alpha Z \mathbf{e}^{(-r)} \sin(\theta)\sin(\phi) - \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \sin(\theta)\cos(\phi)$$

of which we select those parts separately.

```
> rp := Re(rhs(%)) assuming real;
```

$$rp := -\frac{1}{2}\alpha Z \mathbf{e}^{(-r)} \sin(\theta)\sin(\phi)$$

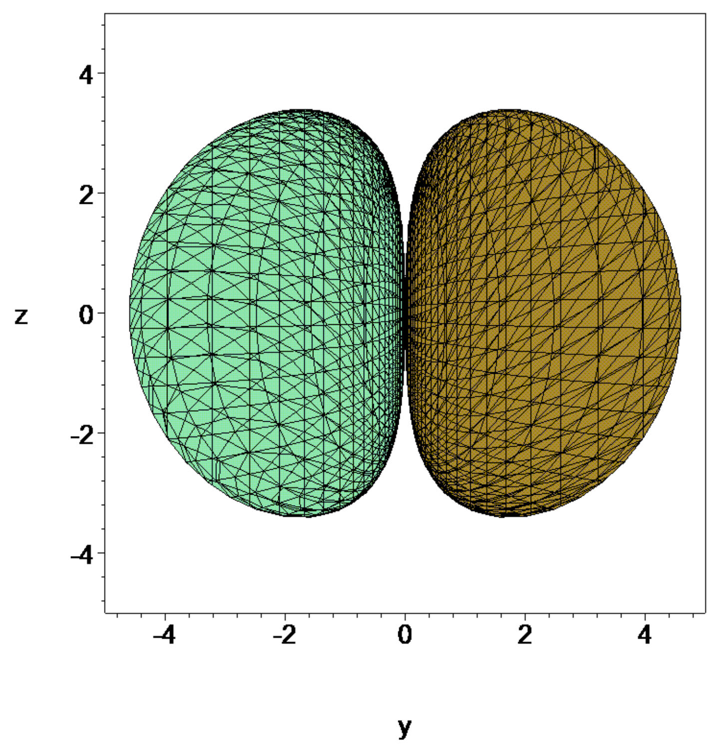
```
> ip := Im(rhs(%%)) assuming real;
```

$$ip := -\frac{1}{2}\alpha Z \mathbf{e}^{(-r)}\sin(\theta)\cos(\phi)$$

We plot the surface itself separately in its real and imaginary parts.

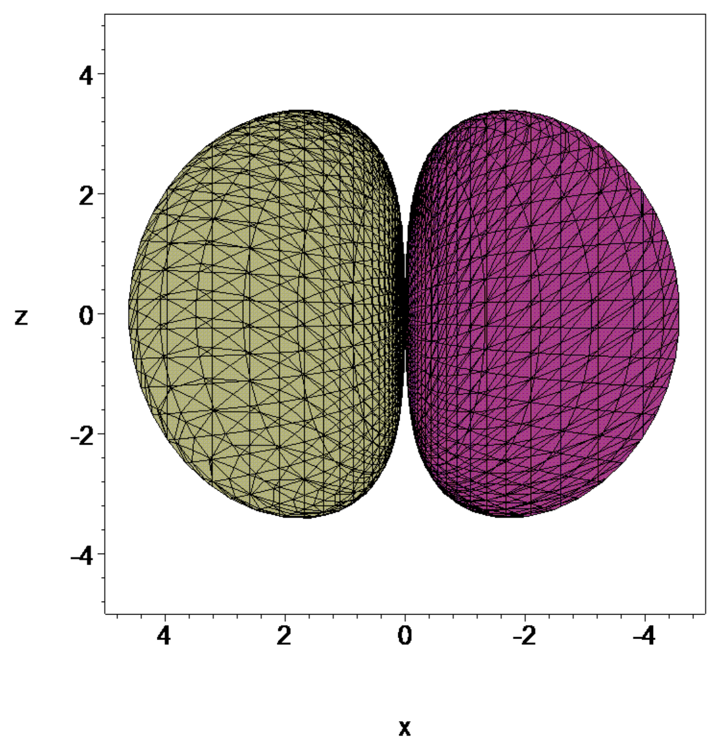
```
> plots[implicitplot3d]([eval(rp, cond)=0.0000365,
     eval(rp, cond)=-0.0000365], r=0..5, theta=0..Pi,
     phi=0..2*Pi, colour=[aquamarine, sienna],
  orientation=[0,90], labels=["x","y","z"],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |1,0,1/2,-1/2>, component 3, real
  part",
     titlefont=[TIMES,BOLD,14], view=[-5..5,-5..5,-5..5]);
```

amplitude function |1,0,1/2,-1/2>, component 3, real part



```
>
> plots[implicitplot3d]([eval(ip, cond)=0.0000365,
    eval(ip, cond)=-0.0000365], r=0..5, theta=0..Pi,
  phi=0..2*Pi,
    labels=["x","y","z"], colour=[maroon, khaki],
  orientation=[90,90],
    coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
    title="amplitude function |1,0,1/2,-1/2>, component 3,
  imaginary part",
    titlefont=[TIMES,BOLD,14], view=[-5..5,-5..5,-5..5]);
```

amplitude function |1,0,1/2,-1/2>, component 3, imaginary part




```
>
```

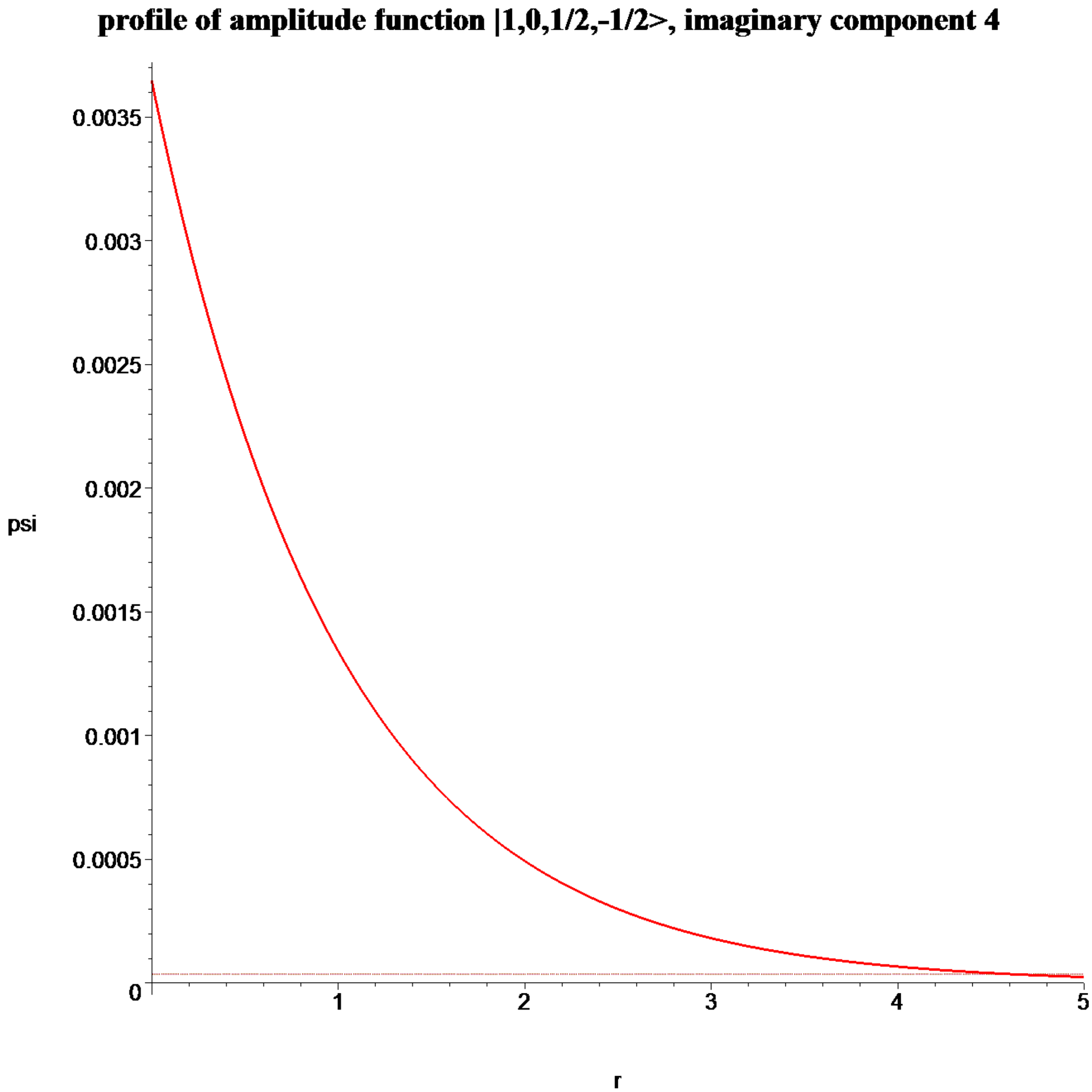
The surfaces in the preceding two plots resemble perfectly the surfaces of the real and imaginary parts of $\psi_{0,\,1,\,1}(r, \theta, \phi)$. Whereas the first component is identically zero, the fourth component is purely imaginary;

```
> '`|1,0,1/2,-1/2>`'[4] = `|1,0,1/2,-1/2>`[4];
```

$$|1,0,1/2,\text{-}1/2>_4 = \frac{1}{2} I\, \alpha\, Z\, \mathbf{e}^{(-r)} \cos(\theta)$$

we plot first the profile along the polar axis, for which $\theta = 0$, to obtain the criterion for the surface,

```
> plot([eval(Im(`|1,0,1/2,-1/2>`[4]), [theta=0,op(cond)]),
  0.0000365], r=0..5,
     title="profile of amplitude function |1,0,1/2,-1/2>,
  imaginary component 4",
     titlefont=[TIMES,BOLD,14], colour=[red, brown],
  linestyle=[1,2],
     labels=["r", "psi"], thickness=[3,2]);
```



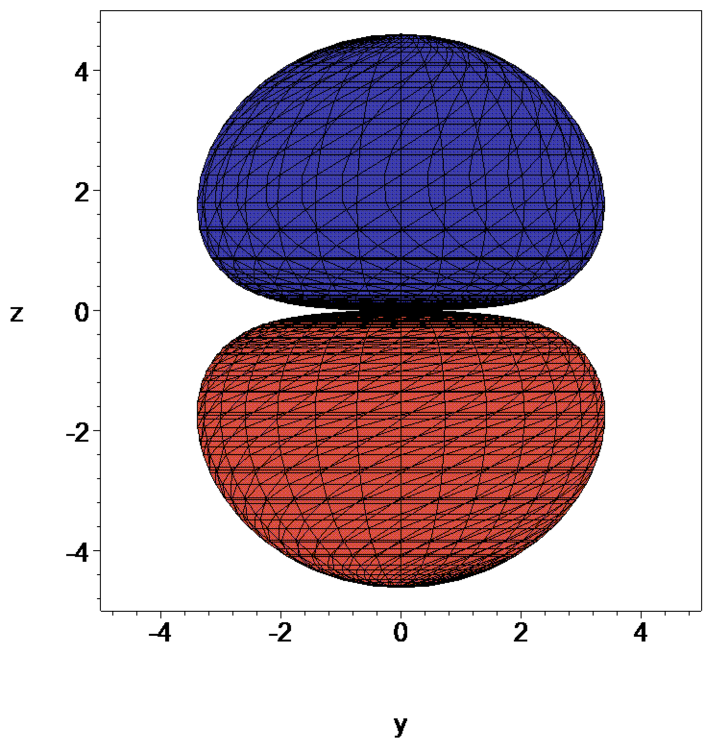
>

and then the surface itself, which we plot.

```
> plots[implicitplot3d]([eval(Im(`|1,0,1/2,-1/2>`[4]),
  cond)=0.0000365,
     eval(Im(`|1,0,1/2,-1/2>`[4]), cond)=-0.0000365], r=0..5,
  theta=0..Pi,
     phi=0..2*Pi, colour=[navy, orange], orientation=[0,90],
  labels=["x","y","z"],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |1,0,1/2,-1/2>, imaginary
  component 4",
```

```
titlefont=[TIMES,BOLD,14], view=[-5..5,-5..5,-5..5]);
```

amplitude function |1,0,1/2,-1/2>, imaginary component 4




```
>
```

This imaginary amplitude function resembles perfectly $\psi_{0,\,1,\,0}(r, \theta, \phi)$ that comprises only a real part. From |1,0,1/2,-1/2>,

```
> p := evalc(`|1,0,1/2,-1/2>`);
```

$$p := \begin{bmatrix} 0 \\ -\mathbf{e}^{(-r)} \\ -\frac{1}{2}\alpha Z \mathbf{e}^{(-r)} \sin(\theta)\sin(\phi) - \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \sin(\theta)\cos(\phi) \\ \frac{1}{2} I \alpha Z \mathbf{e}^{(-r)} \cos(\theta) \end{bmatrix}$$

and its complex conjugate,

```
> pc := evalc(subs(I=-I,`|1,0,1/2,-1/2>`));
```

$$pc := \left[\begin{array}{c} 0 \\ -e^{(-r)} \\ -\frac{1}{2}\alpha Z e^{(-r)} \sin(\theta)\sin(\phi) + \frac{1}{2} I \alpha Z e^{(-r)} \sin(\theta)\cos(\phi) \\ \frac{-1}{2} I \alpha Z e^{(-r)} \cos(\theta) \end{array}\right]$$

we form scalar product |1,0,1/2,-1/2>* . |1,0,1/2,-1/2>,

```
> ps := 
  simplify(evalc(expand(subs(I=-I,LinearAlgebra:-Transpose(`|1,0,
  1/2,-1/2>`)) . `|1,0,1/2,-1/2>`)));
```

$$ps := \frac{1}{4} e^{(-2\,r)} (Z^2 \alpha^2 + 4)$$

which we separate into the two parts,

```
> fl := simplify(remove(has, expand(ps), alpha));
```

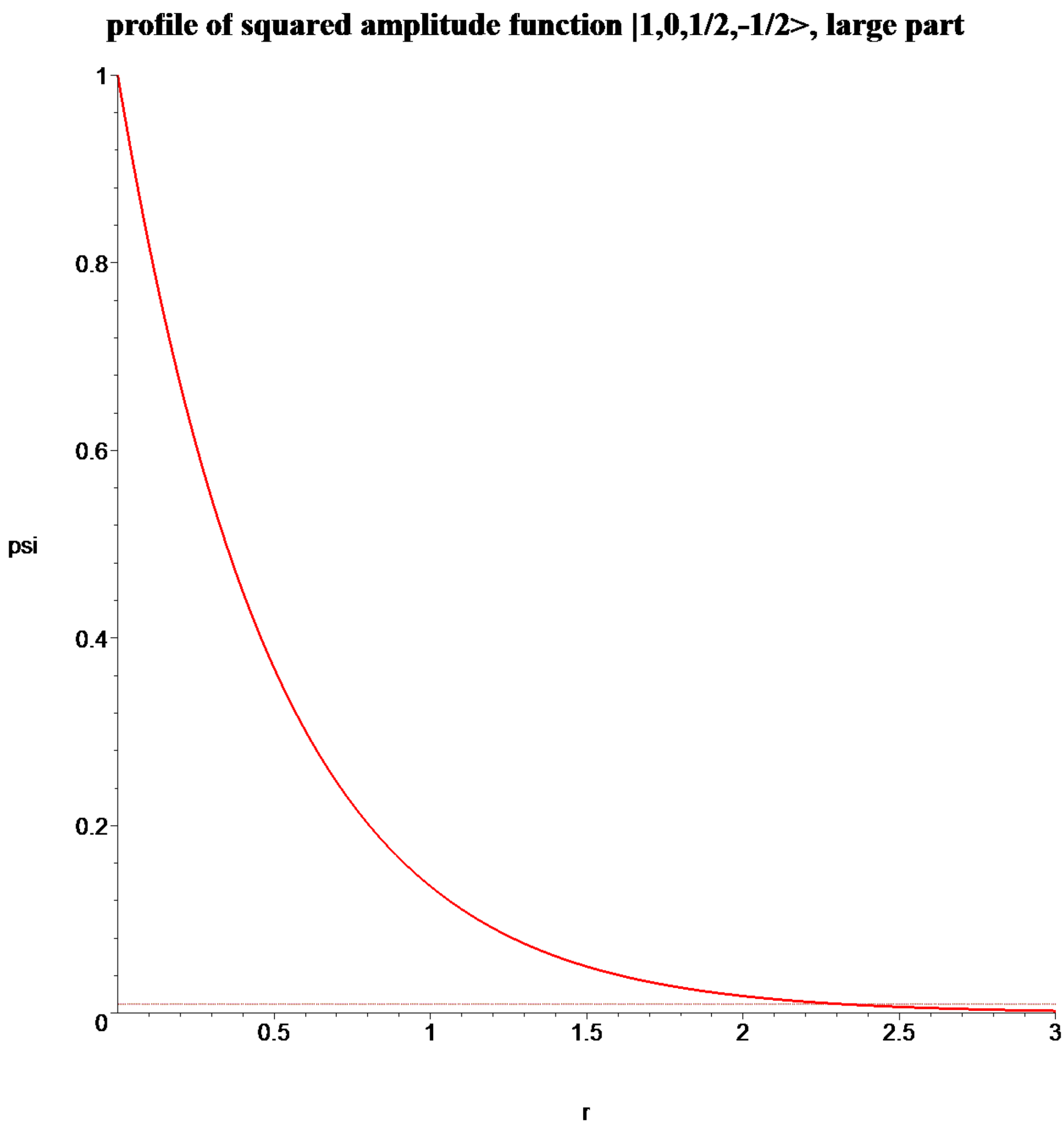
$$fl := e^{(-2\,r)}$$

```
> fs := simplify(ps - fl);
```

$$fs := \frac{1}{4} e^{(-2\,r)} Z^2 \alpha^2$$

and plot the profile of its part that does not contain α.

```
> plot([eval(fl, cond), 0.01], r=0..3, 0..1,
     title="profile of squared amplitude function |1,0,1/2,-1/2>,
  large part",
     titlefont=[TIMES,BOLD,14], colour=[red, brown],
  linestyle=[1,2],
     labels=["r", "psi"], thickness=[3,2]);
```

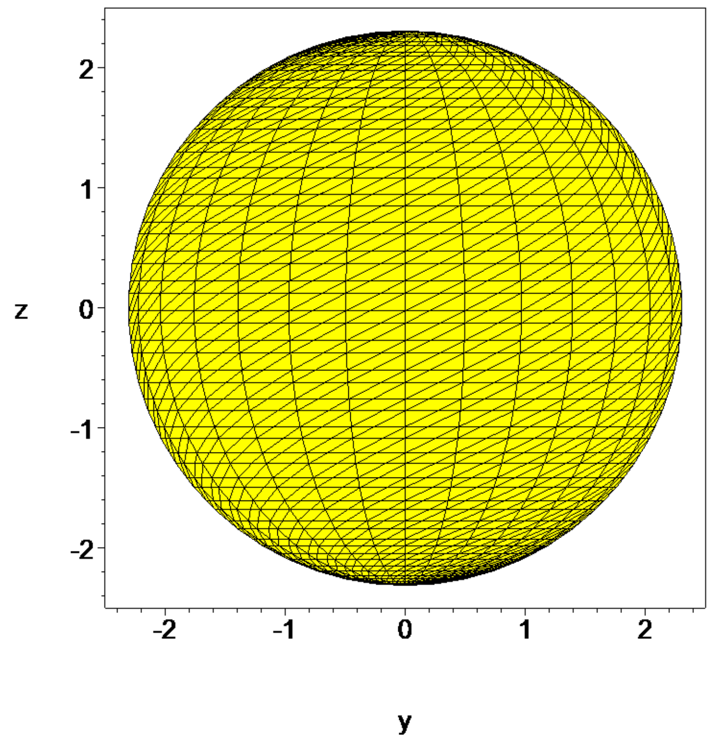



```
>
```

For that large part of |1,0,1/2,-1/2> squared we plot its surface,

```
> plots[implicitplot3d](eval(fl, cond)=0.01, r=0..5, theta=0..Pi,
   phi=0..2*Pi, colour=yellow, orientation=[0,90],
 labels=["x","y","z"],
   coords = scispherical, grid=[30,30,30], scaling=constrained,
 axes=box,
   title="squared amplitude function |1,0,1/2,-1/2>, large
 part",
   titlefont=[TIMES,BOLD,14],
 view=[-2.5..2.5,-2.5..2.5,-2.5..2.5]);
```

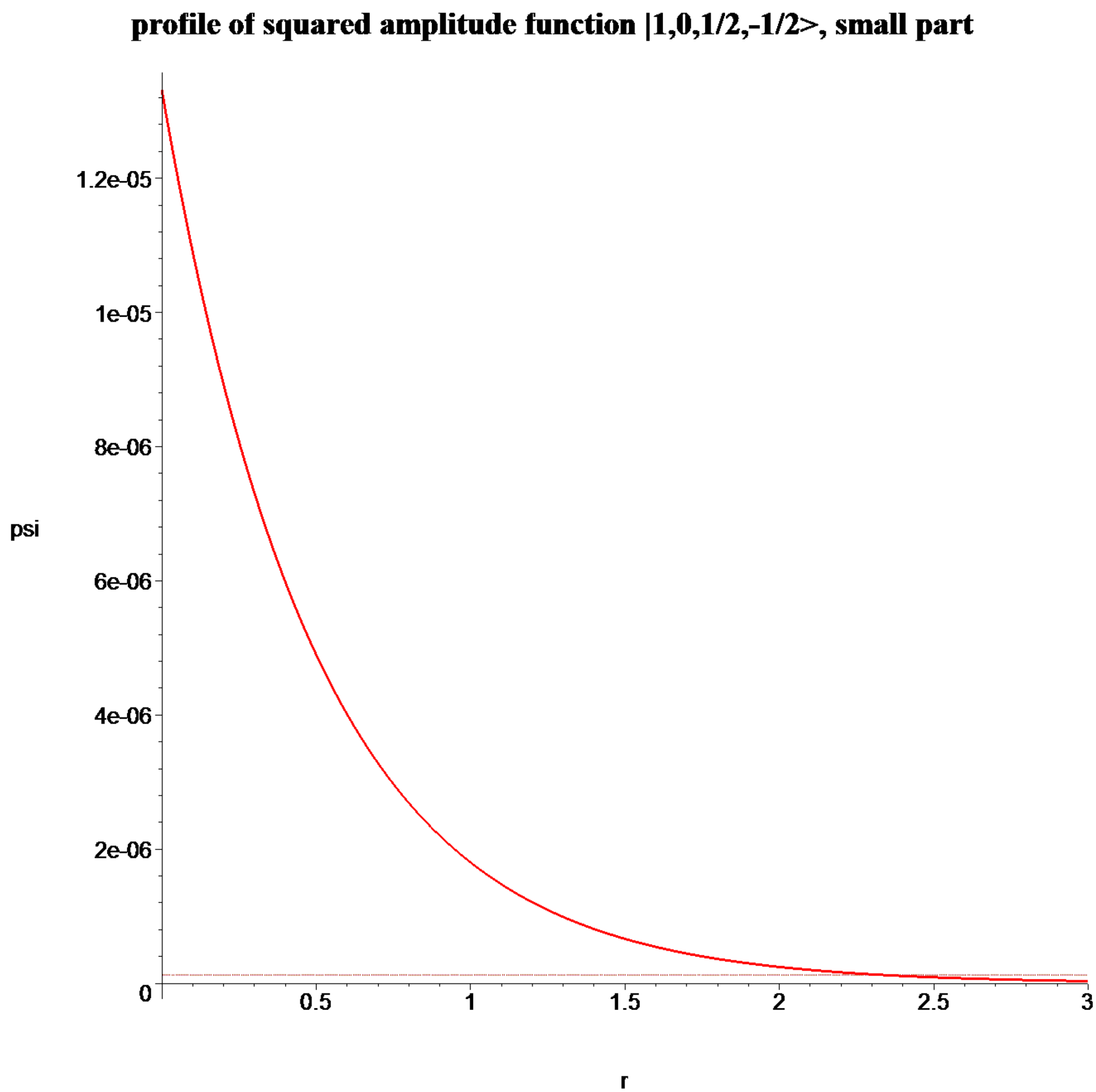
squared amplitude function |1,0,1/2,-1/2>, large part



\>

which yields a perfect sphere, as expected from term $\mathbf{e}^{(-2\,r)}$; for the small part of the square, we obtain this profile along the polar axis.

```
> plot([eval(fs, [op(cond), theta=0, phi=0]), 1.2e-7], r=0..3,
     title="profile of squared amplitude function |1,0,1/2,-1/2>,
  small part",
     titlefont=[TIMES,BOLD,14], colour=[red, brown],
  linestyle=[1,2],
     labels=["r", "psi"], thickness=[3,2]);
```

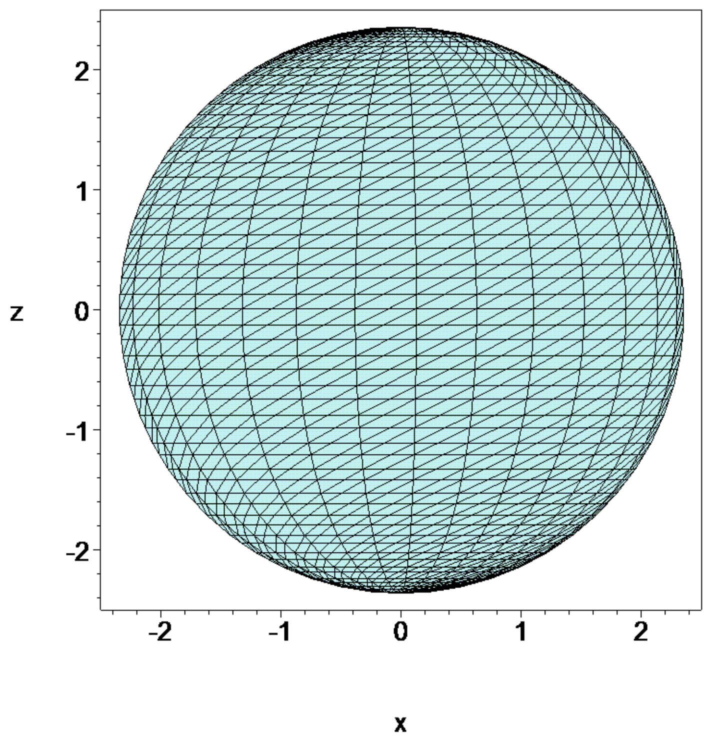


>

We accordingly plot the surface of the small part of |1,0,1/2,-1/2> squared,

```
> plots[implicitplot3d](eval(fs, cond)=1.2e-7, r=0..3.5,
  theta=0..Pi, phi=0..2*Pi,
     colour=turquoise, axes=box, orientation=[-90,90],coords =
  scispherical,
     grid=[30,30,30], scaling=constrained,
  view=[-2.5..2.5,-2.5..2.5,-2.5..2.5],
     title="squared amplitude function |1,0,1/2,-1/2>, small
  part",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14]);
```

squared amplitude function |1,0,1/2,-1/2>, small part




```
>
```

These surfaces of the large and small parts of squared |1,0,1/2,-1/2> have the same diameter. The profiles and surfactes of these two eigenfunctions |1,0,1/2,1/2> and |1,0,1/2,-1/2>, which differ only in their equatorial quantum numbers $m = \frac{1}{2}$ and $m = -\frac{1}{2}$, have notably similar graphical characteristics.; comparison of these two eigenfunctions above indicates that differences between them are only a different ordering of the components and a reversal of phase.

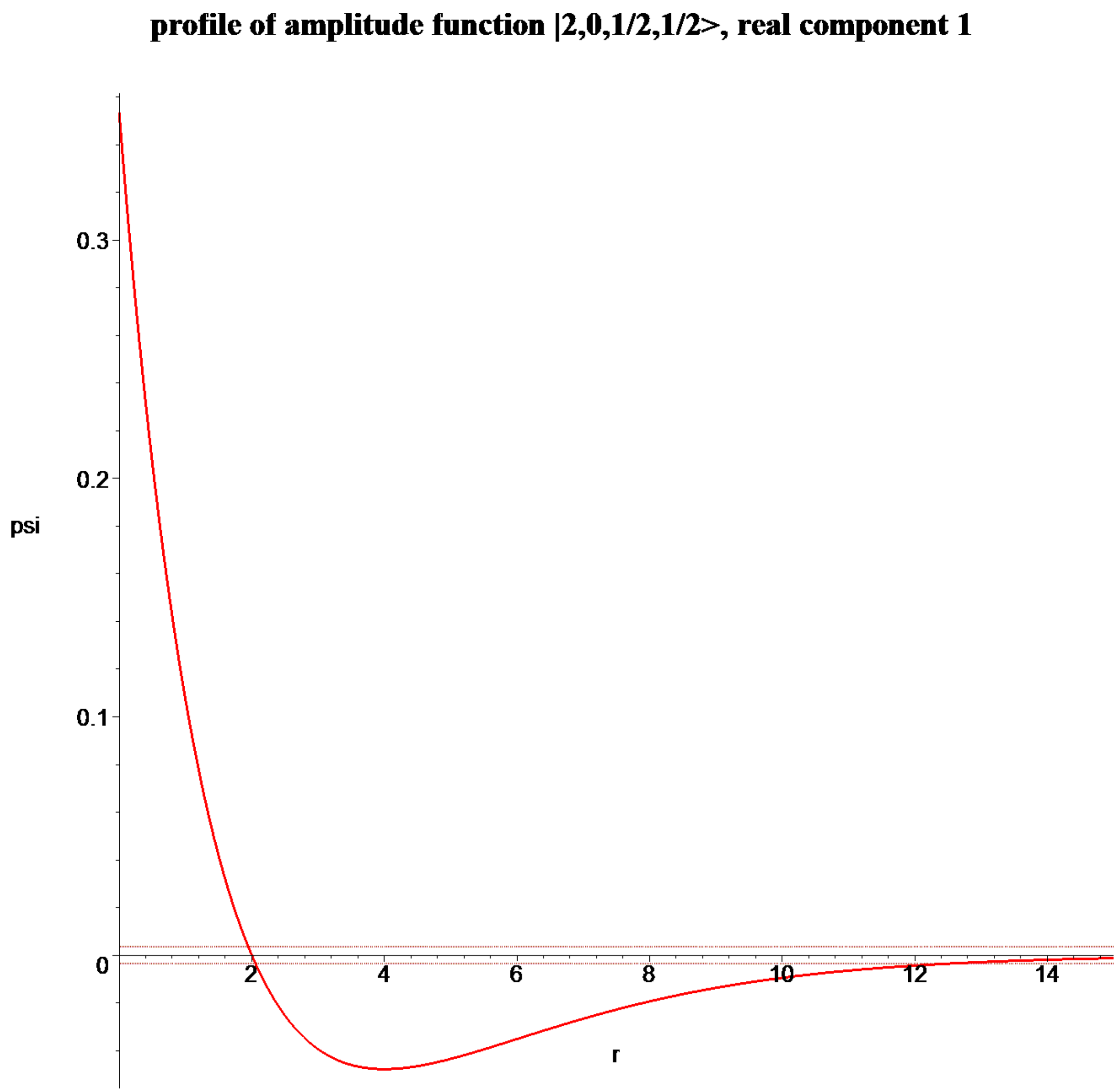
We investigate |2,0,1/2,1/2> analogously.

```
> '`|2,0,1/2,1/2>`' = `|2,0,1/2,1/2>`;
```

$$|2,0,1/2,1/2\rangle = \begin{bmatrix} \frac{1}{4}\sqrt{2}\left(1-\frac{r}{2}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)} \\ 0 \\ \frac{1}{8}I\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)}\cos(\theta) \\ \frac{1}{8}I\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\,\mathbf{e}^{(\phi I)} \end{bmatrix}$$

We plot the radial profile of the first component of |2,0,1/2,1/2>.

```
> plot([`|2,0,1/2,1/2>`[1], 0.0035, -0.0035], r=0..15,
    title="profile of amplitude function |2,0,1/2,1/2>, real
  component 1",
    titlefont=[TIMES,BOLD,14], colour=[red, brown, brown],
  linestyle=[1,2,2],
    labels=["r", "psi"], thickness=[3,2,2]);
```



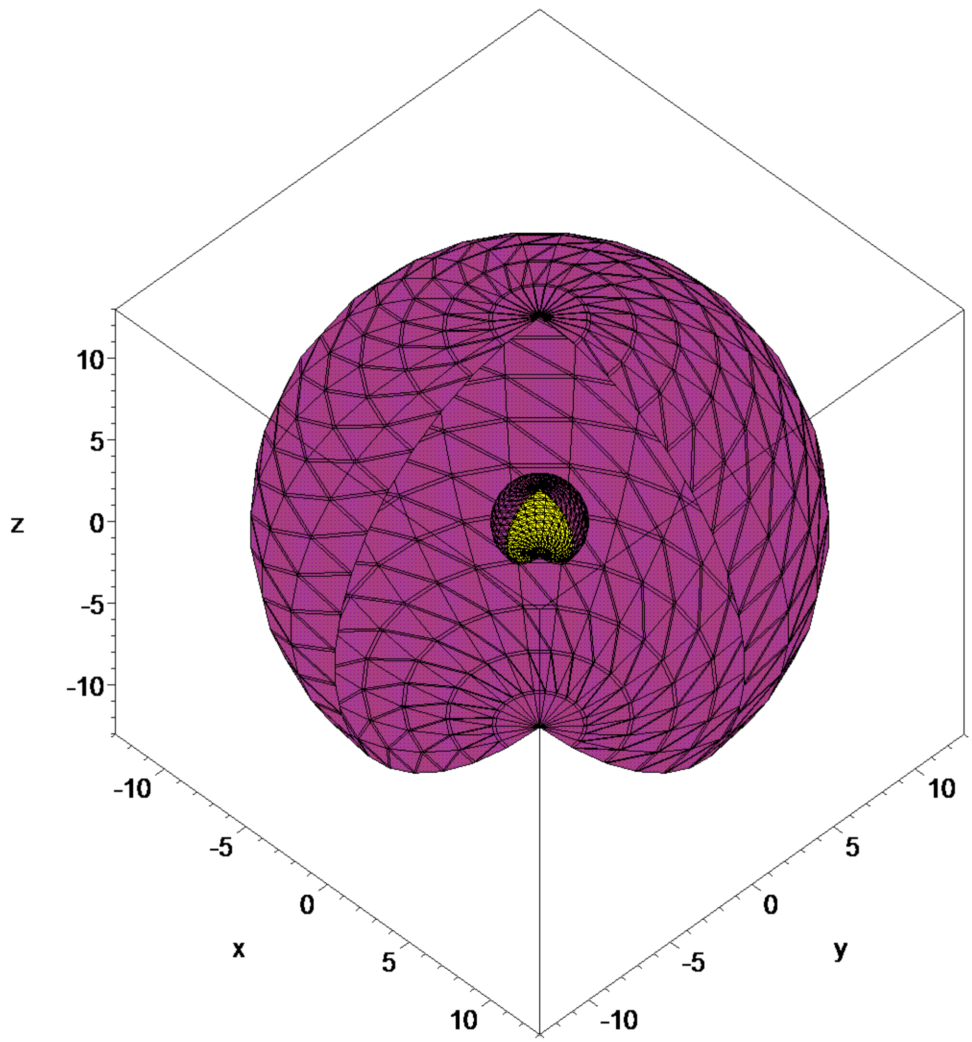

```
>
```

We plot the surface of this first component of |2,0,1/2,1/2> at a value of ψ that is $\frac{1}{100}$ of its maximum value, cut open to show the inner lobe,

```
> plots[implicitplot3d]([`|2,0,1/2,1/2>`[1]=0.0035,
  `|2,0,1/2,1/2>`[1]=-0.0035],
     r=0..15, theta=0..Pi, phi=0..3/2*Pi, colour=[yellow,
  maroon], labels=["x","y","z"],
     coords = scispherical, grid=[20,20,20], scaling=constrained,
  axes=box,
     title="amplitude function |2,0,1/2,1/2>, real component 1",
  orientation=[-45,45],
```

```
titlefont=[TIMES,BOLD,14], view=[-13..13,-13..13,-13..13]);
```

amplitude function |2,0,1/2,1/2>, real component 1



>

which generates three concentric perfect spheres because this component has no angular dependence; this surface is practically identical with that of $\psi_{1,0,0}(r, \theta, \phi)$ in spherical polar coordinates. The second component of |2,0,1/2,1/2> is zero; the third component is purely imaginary;

```
> '`|2,0,1/2,1/2>`'[3] = `|2,0,1/2,1/2>`[3];
```

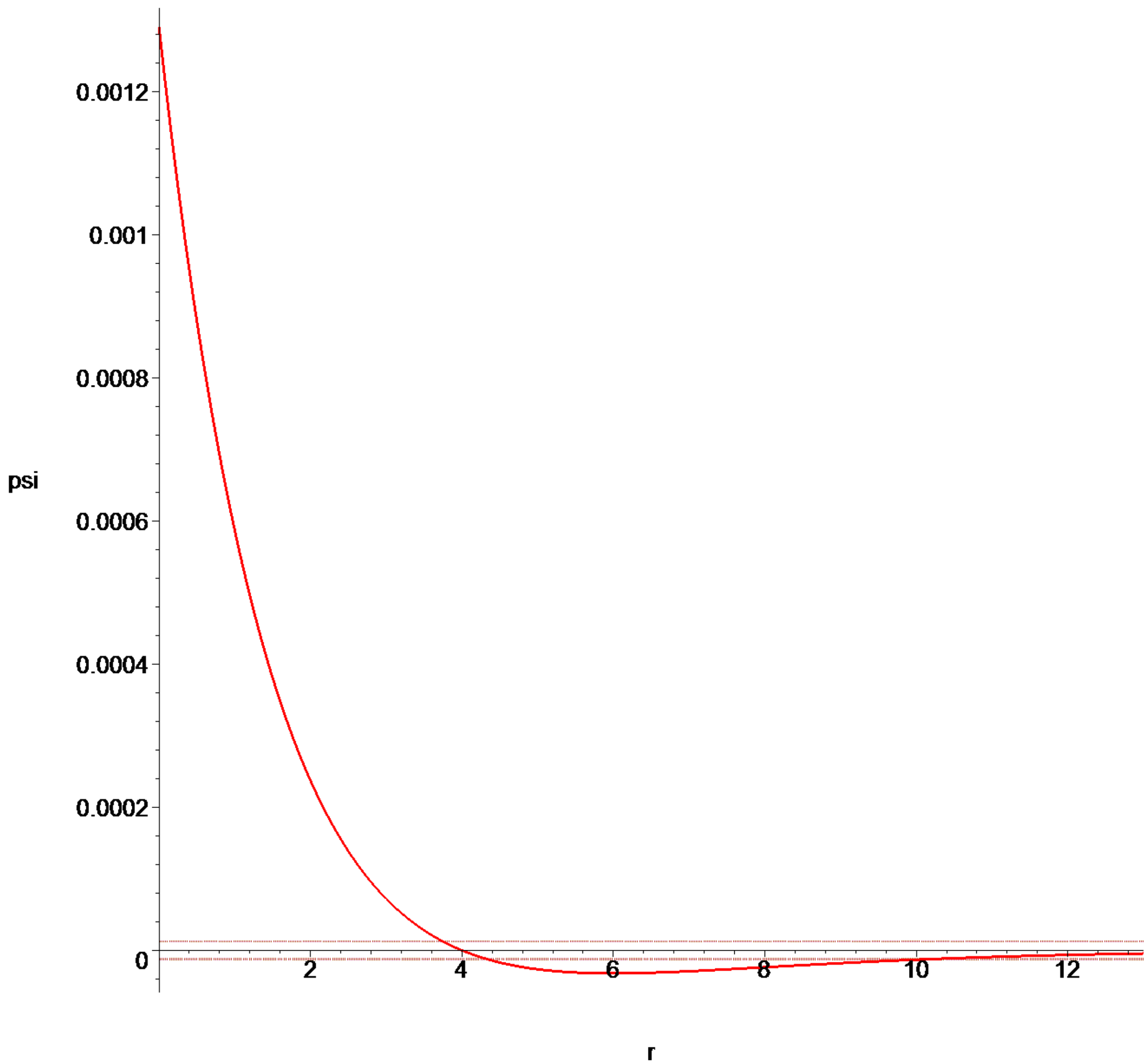
$$|2,0,1/2,1/2>_3 = \frac{1}{8} I \sqrt{2}\, \alpha\, Z \left(1 - \frac{r}{4}\right) \mathbf{e}^{\left(-\frac{r}{2}\right)} \cos(\theta)$$

we plot first the profile along the polar axis, for which $\theta = 0$, to obtain the criterion for the surface,

```
> plot([eval(Im(`|2,0,1/2,1/2>`[3]), [theta=0,op(cond)]),
```

```
0.0000125, -0.0000125],
    r=0..13, titlefont=[TIMES,BOLD,14], colour=[red, brown,
brown],
    title="profile of amplitude function |2,0,1/2,1/2>,
imaginary component 3",
    linestyle=[1,2,2], labels=["r", "psi"], thickness=[3,2]);
```

profile of amplitude function |2,0,1/2,1/2>, imaginary component 3



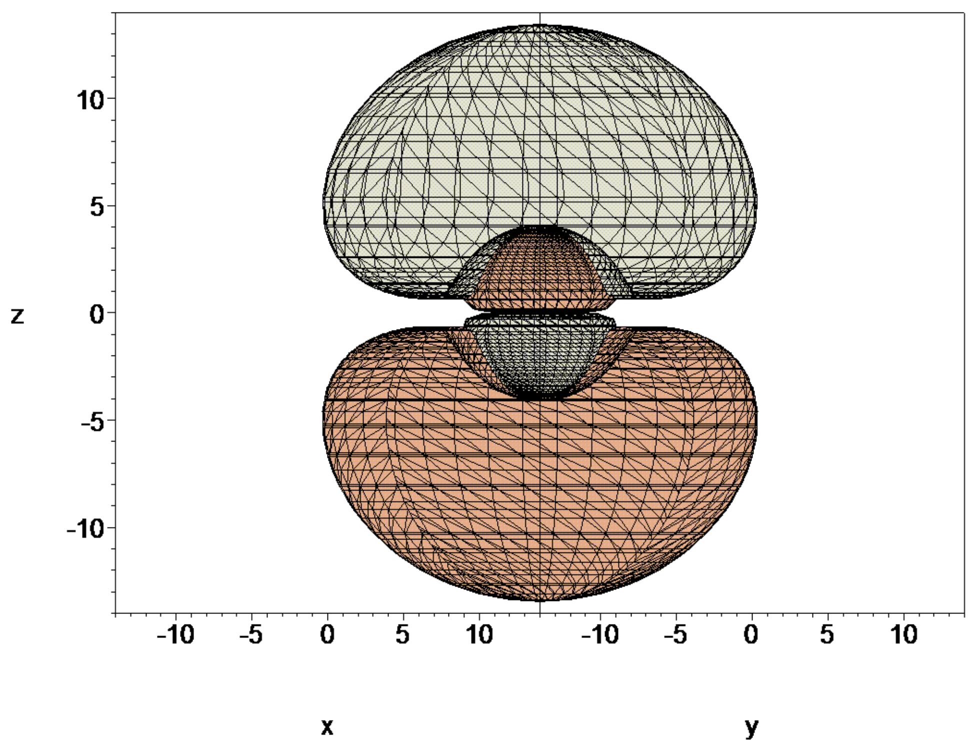
>

and then the surface itself.

```
> plots[implicitplot3d]([eval(Im(`|2,0,1/2,1/2>`[3]),
cond)=0.00000365,
   eval(Im(`|2,0,1/2,1/2>`[3]), cond)=-0.00000365], r=0..15,
theta=0..Pi,
```

```
   phi=0..3/2*Pi, colour=[tan, wheat], orientation=[-45,90],
labels=["x","y","z"],
   coords = scispherical, grid=[30,30,30], scaling=constrained,
axes=box,
   title="amplitude function |2,0,1/2,1/2>, imaginary component
3",
   titlefont=[TIMES,BOLD,14], view=[-14..14,-14..14,-14..14]);
```

amplitude function |2,0,1/2,1/2>, imaginary component 3



>

This surface is practically identical with that of $\psi_{1,\,1,\,0}(r, \theta, \phi)$ in spherical polar coordinates. The fourth component has both real and imaginary parts,

```
> '`|2,0,1/2,1/2>`'[4] = evalc(`|2,0,1/2,1/2>`[4]);
```

$|2,0,1/2,1/2>_4 =$

$$-\frac{1}{8}\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\sin(\phi)+\frac{1}{8}I\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\phi)$$

of which we select those parts separately.

```
> rp := Re(rhs(%)) assuming real;
```

$$rp:=-\frac{1}{8}\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\sin(\phi)$$

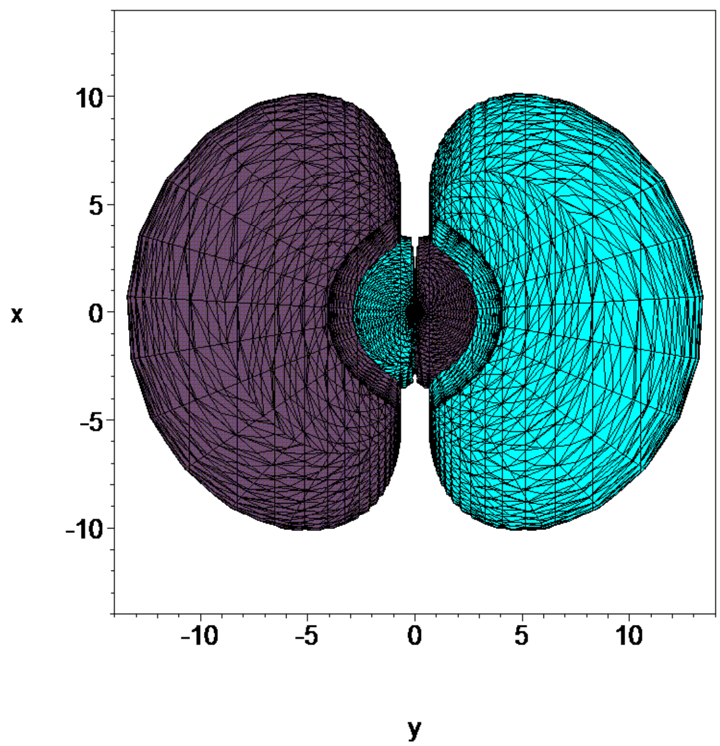
```
> ip := Im(rhs(%%)) assuming real;
```

$$ip:=\frac{1}{8}\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\phi)$$

We plot the surfaces in their real and imaginary parts cut open to expose the inner lobes.

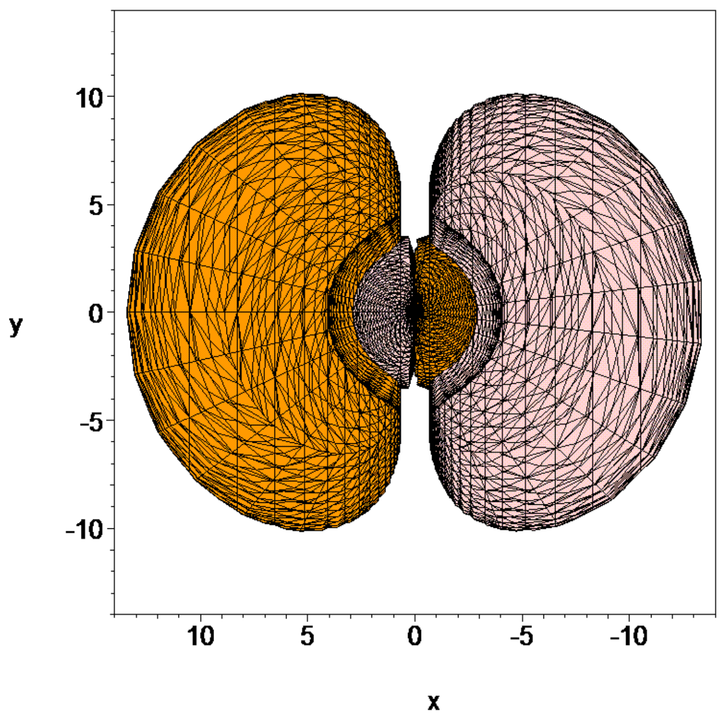
```
> plots[implicitplot3d]([eval(rp, cond)=0.00000365,
    eval(rp, cond)=-0.00000365], r=0..15, theta=0..3/4*Pi,
    phi=0..2*Pi, colour=[cyan, violet], orientation=[0,180],
  labels=["x","y","z"],
    coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
    title="amplitude function |2,0,1/2,1/2>, component 4, real
  part",
    titlefont=[TIMES,BOLD,14], view=[-14..14,-14..14,-14..14]);
```

amplitude function |2,0,1/2,1/2>, component 4, real part




```
>
> plots[implicitplot3d]([eval(ip, cond)=0.00000365,
    eval(ip, cond)=-0.00000365], r=0..15, theta=0..3/4*Pi,
  phi=0..2*Pi,
    labels=["x","y","z"], colour=[pink, coral],
  orientation=[90,180],
    coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
    title="amplitude function |2,0,1/2,1/2>, component 4,
  imaginary part",
    titlefont=[TIMES,BOLD,14], view=[-14..14,-14..14,-14..14]);
```

amplitude function |2,0,1/2,1/2>, component 4, imaginary part




```
>
```

The latter three surfaces resemble those of $\psi_{1,1,0}(r, \theta, \phi)$ symmetric about the polar axis or rotated to become symmetric about the other two axes, equivalent to the real and imaginary parts of $\psi_{1,1,1}(r, \theta, \phi)$. From |2,0,1/2,1/2>,

```
> p := evalc(`|2,0,1/2,1/2>`);
```

$$p := \begin{bmatrix} \frac{1}{4}\sqrt{2}\left(1-\frac{r}{2}\right)e^{\left(-\frac{r}{2}\right)} \\ 0 \\ \frac{1}{8}I\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)e^{\left(-\frac{r}{2}\right)}\cos(\theta) \\ -\frac{1}{8}\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)e^{\left(-\frac{r}{2}\right)}\sin(\theta)\sin(\phi)+\frac{1}{8}I\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)e^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\phi) \end{bmatrix}$$

and its complex conjugate,

```
> pc := evalc(subs(I=-I,`|2,0,1/2,1/2>`));
```

$$pc := \begin{bmatrix} \frac{1}{4}\sqrt{2}\left(1-\frac{r}{2}\right)e^{\left(-\frac{r}{2}\right)} \\ 0 \\ \frac{-1}{8}I\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)e^{\left(-\frac{r}{2}\right)}\cos(\theta) \\ -\frac{1}{8}\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)e^{\left(-\frac{r}{2}\right)}\sin(\theta)\sin(\phi)-\frac{1}{8}I\sqrt{2}\,\alpha\,Z\left(1-\frac{r}{4}\right)e^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\phi) \end{bmatrix}$$

we form scalar product |2,0,1/2,1/2>* **.** |2,0,1/2,1/2>,

```
> ps :=
  simplify(evalc(subs(I=-I,LinearAlgebra:-Transpose(`|2,0,1/2,1/2
  >`)) . `|2,0,1/2,1/2>`)) assuming real;
```

$$ps := \frac{1}{512}e^{(-r)}(Z^2\alpha^2 r^2 - 8Z^2\alpha^2 r + 16Z^2\alpha^2 + 16r^2 - 64r + 64)$$

We separate the terms according to their content.

```
> fl := remove(has, expand(ps), alpha);
```

$$fl := \frac{1}{32}\frac{r^2}{e^r} - \frac{1}{8}\frac{r}{e^r} + \frac{1}{8}\frac{1}{e^r}$$

```
> fs := simplify(ps - fl);
```

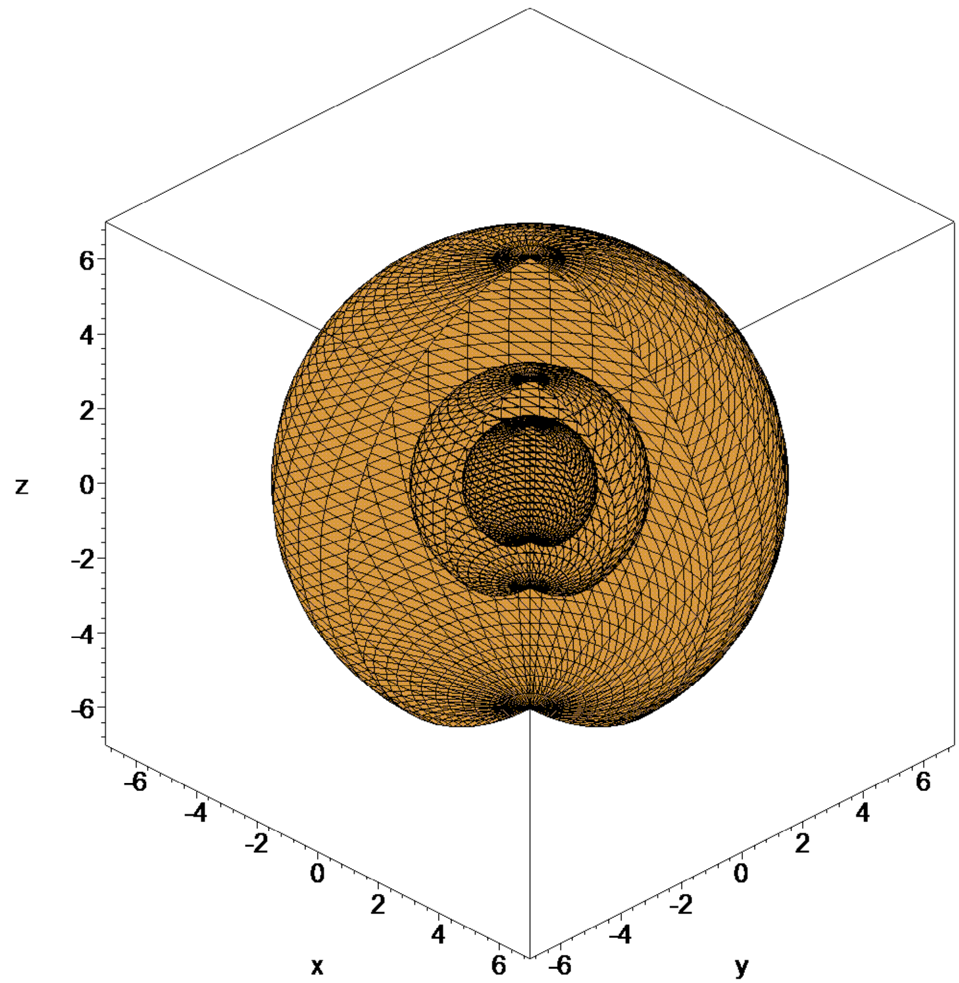
$$fs := \frac{1}{512}e^{(-r)}Z^2\alpha^2(-4+r)^2$$

of which there are no angular contributions in either case. For that large part of |2,0,1/2,1/2> squared we plot its surface, cut open to reveal the inner lobe,

```
> plots[implicitplot3d](eval(fl, cond)=0.00122, r=0..9,
  theta=0..Pi,
     phi=0..3/2*Pi, colour=gold, orientation=[-45,60],
  labels=["x","y","z"],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
```

```
   title="squared amplitude function |2,0,1/2,1/2>, large
part",
   titlefont=[TIMES,BOLD,14], view=[-7..7,-7..7,-7..7]);
```

squared amplitude function |2,0,1/2,1/2>, large part



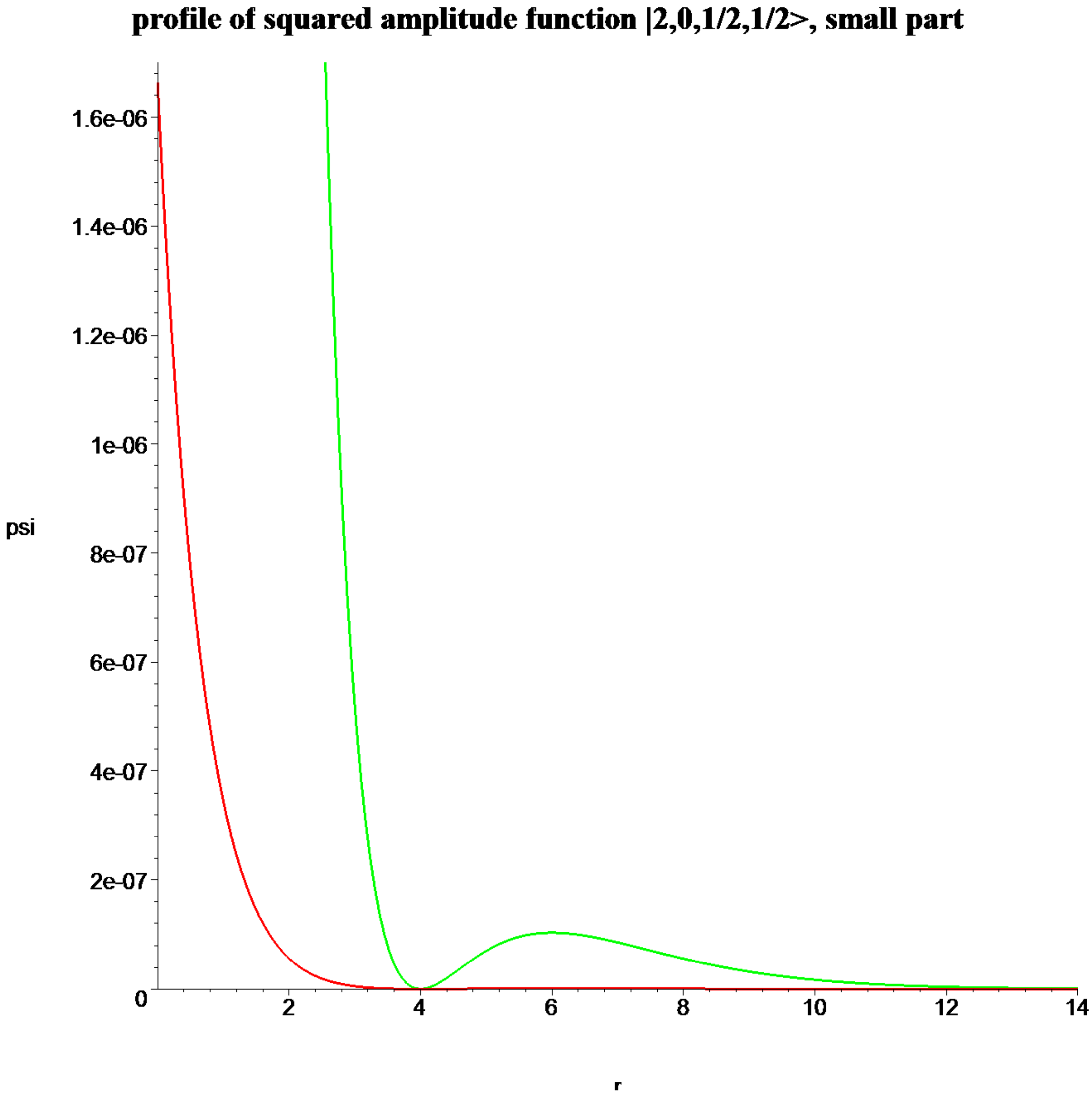
>

which yields three perfectly concentric spheres at distances from the origin corresponding to the three intersections of the red curve in the profile above with the brown line; from the small part of the squared amplitude function, we obtain this profile along the polar axis, red curve, and the same quantity multiplied by 100, green curve, to show that the red curve has an extremum about $r = 4$ units.

```
> plot([eval(fs, cond), 100*eval(fs, cond)], r=0..14, 0..1.7e-6,

   title="profile of squared amplitude function |2,0,1/2,1/2>,
```

```
small part",
   titlefont=[TIMES,BOLD,14], colour=[red, green, brown],
linestyle=[1,1,2],
   labels=["r", "psi"], thickness=[3,3,2]);
```



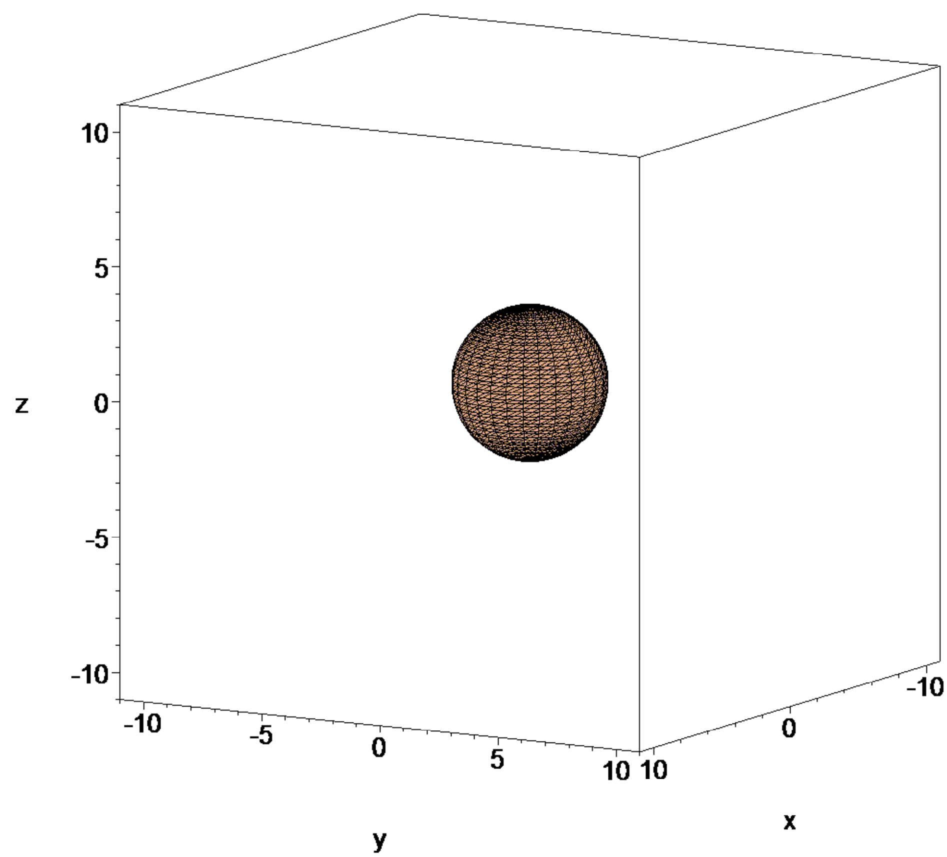

```
>
```

We accordingly plot the surface of the small part of |2,0,1/2,1/2> squared, showing first the inner surface at the standard criterion of ψ,

```
> pl1 := plots[implicitplot3d](eval(fs, cond)=8.3e-9, r=0..11,
theta=0..Pi, phi=0..2*Pi,
   colour=tan, orientation=[30,80],coords = scispherical,
grid=[30,30,30], scaling=constrained,
   axes=box, title="squared amplitude function |2,0,1/2,1/2>,
```

```
small part, inner surface",
   labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
view=[-11..11,-11..11,-11..11]):  pl1;
```

squared amplitude function |2,0,1/2,1/2>, small part, inner surface



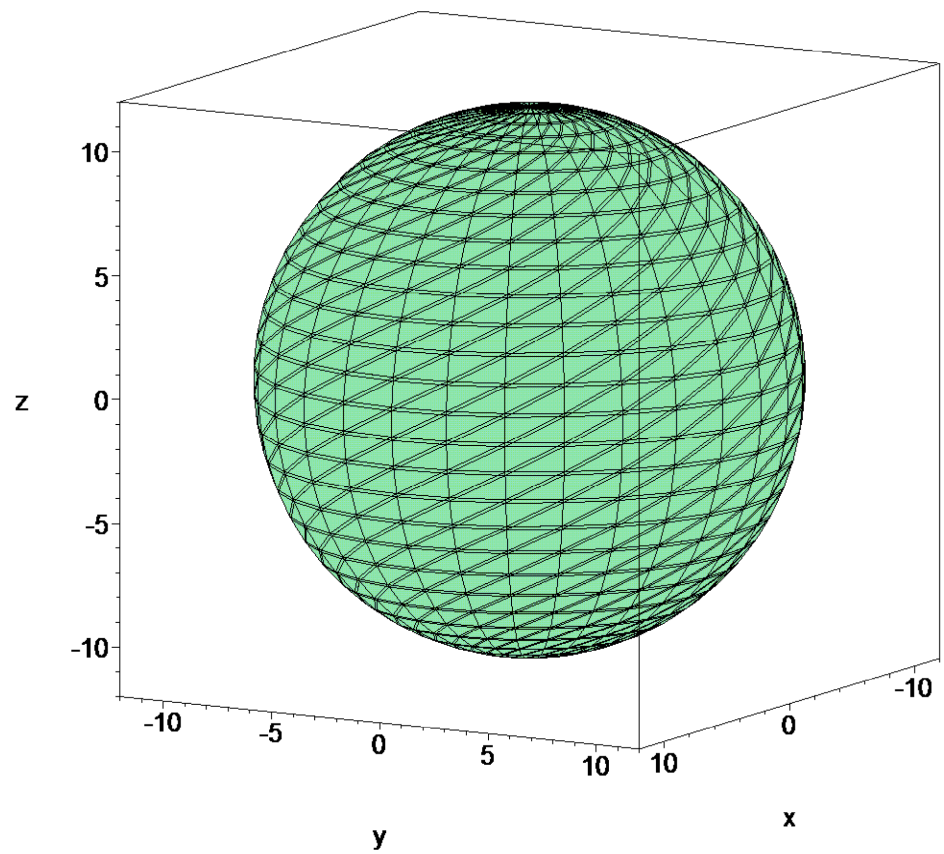
>

which shows only the inner lobe; when we decrease the criterion for the surface to be less than the secondary extremum near $r = 6$, we see the outer surface,

```
> pl2 := plots[implicitplot3d](eval(fs, cond)=8.3e-11, r=0..19,
theta=0..Pi, phi=0..2*Pi,
   colour=aquamarine, orientation=[30,80], coords =
scispherical, grid=[30,30,30], scaling=constrained,
   axes=box, title="squared amplitude function |2,0,1/2,1/2>,
small part, outer surface",
```

```
   labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
  view=[-12..12,-12..12,-12..12]):  pl2;
```

squared amplitude function |2,0,1/2,1/2>, small part, outer surface

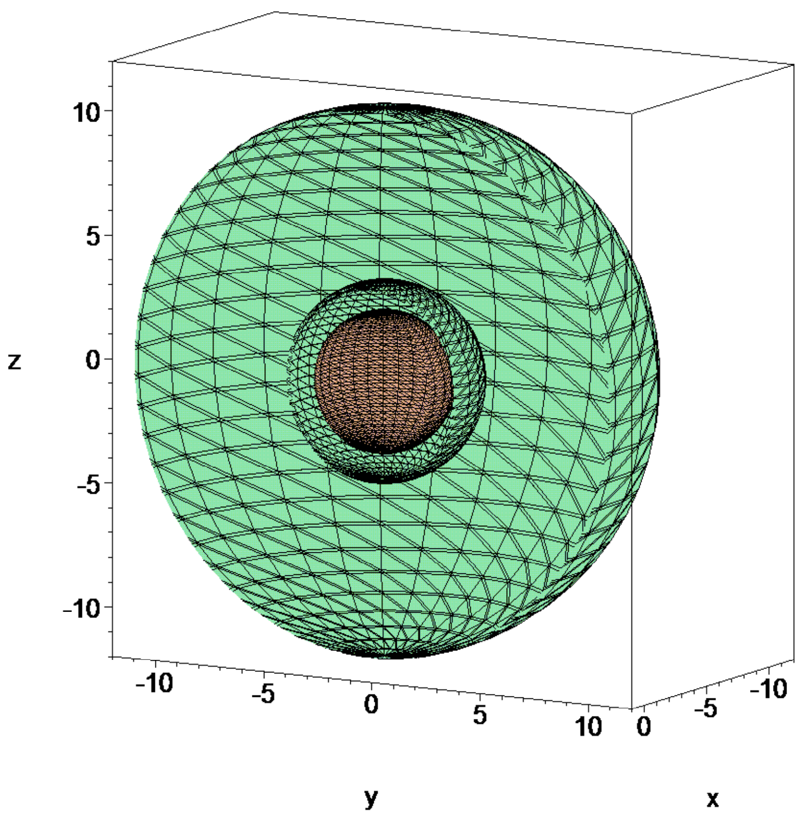



```
>
```

and with the outer surface cut open to reveal the inner lobe.

```
> plots[display](pl1, pl2, labels=["x","y","z"],
  view=[-12..1,-12..12,-12..12],
     title="squared amplitude function |2,0,1/2,1/2>, small
  part",
      titlefont=[TIMES,BOLD,14]);
```

squared amplitude function |2,0,1/2,1/2>, small part

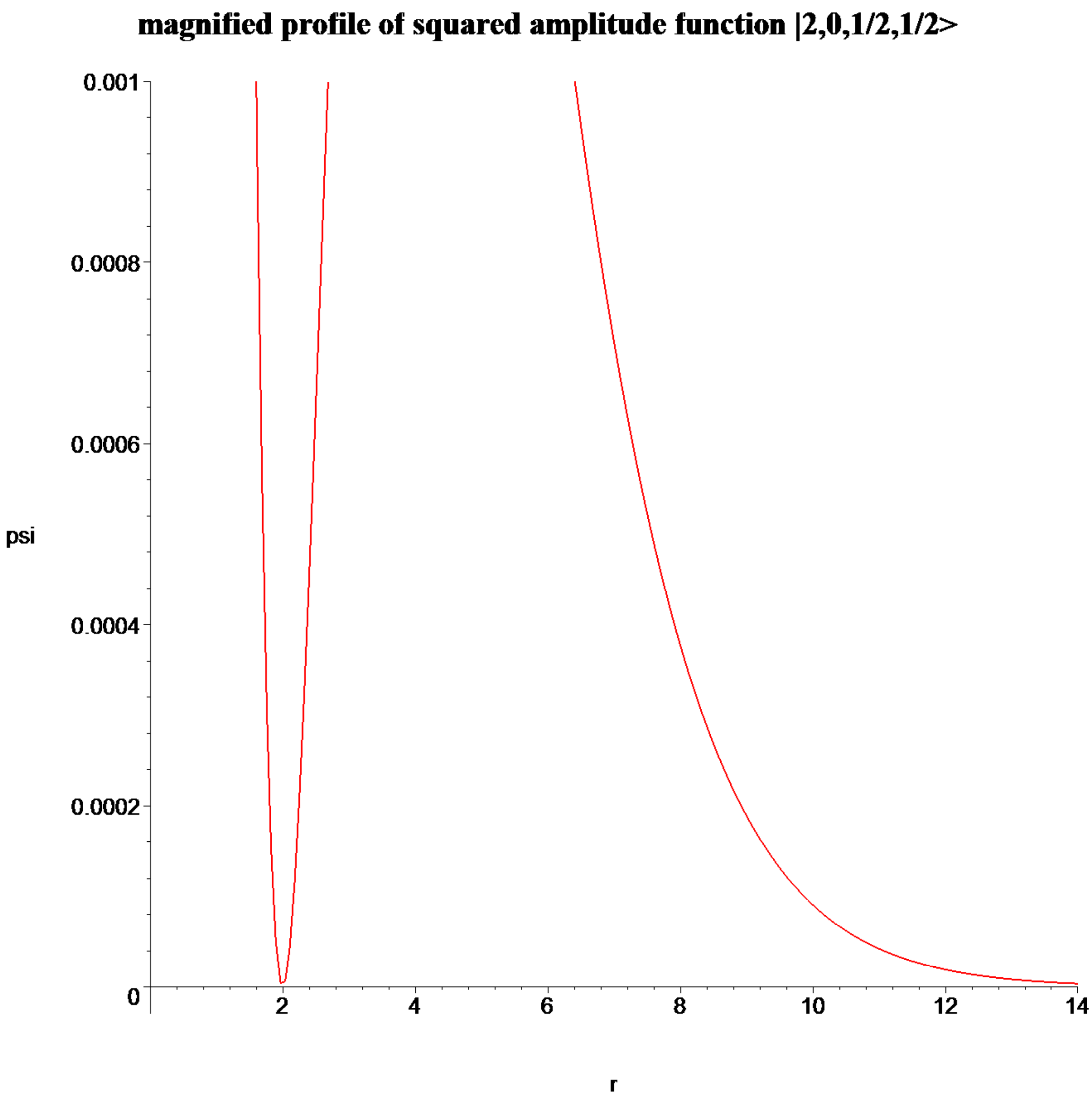



```
>
```

The latter three plots demonstrate the inner lobe of this small component of |2,0,1/2,1/2> squared, which like the real part of |2,0,1/2,1/2> squared resembles $\psi_{1,0,0}(r, \theta, \phi)^2$. When we expand the scale for the sum of the real large and small parts,

```
> plot(eval(fl + fs, cond), r=0..14, -3.0e-5..1.0e-3,
     title="magnified profile of squared amplitude function
  |2,0,1/2,1/2>",
     titlefont=[TIMES,BOLD,14], colour=[red, brown], linestyle=1,

     labels=["r", "psi"], thickness=2, resolution=2000);
```



\>

we see that the curve of the sum of the large and small parts of the squared amplitude function does not osculate the abscissal axis, unlike the radial nodal behaviour of $\psi_{1,\,0,\,0}(r,\,\theta,\,\phi)^2$ from Schroedinger's temporally independent equation in spherical polar coordinates. Hence, although each component of this amplitude function has a radial node, the squared total amplitude function has no such radial node. We expect that the characteristics of the plots of |2,0,1/2,-1/2> resemble those of the corresponding plots of |2,0,1/2,1/2> similarly to the conditions between |1,0,1/2,1/2> and |1,0,1/2,-1/2>.

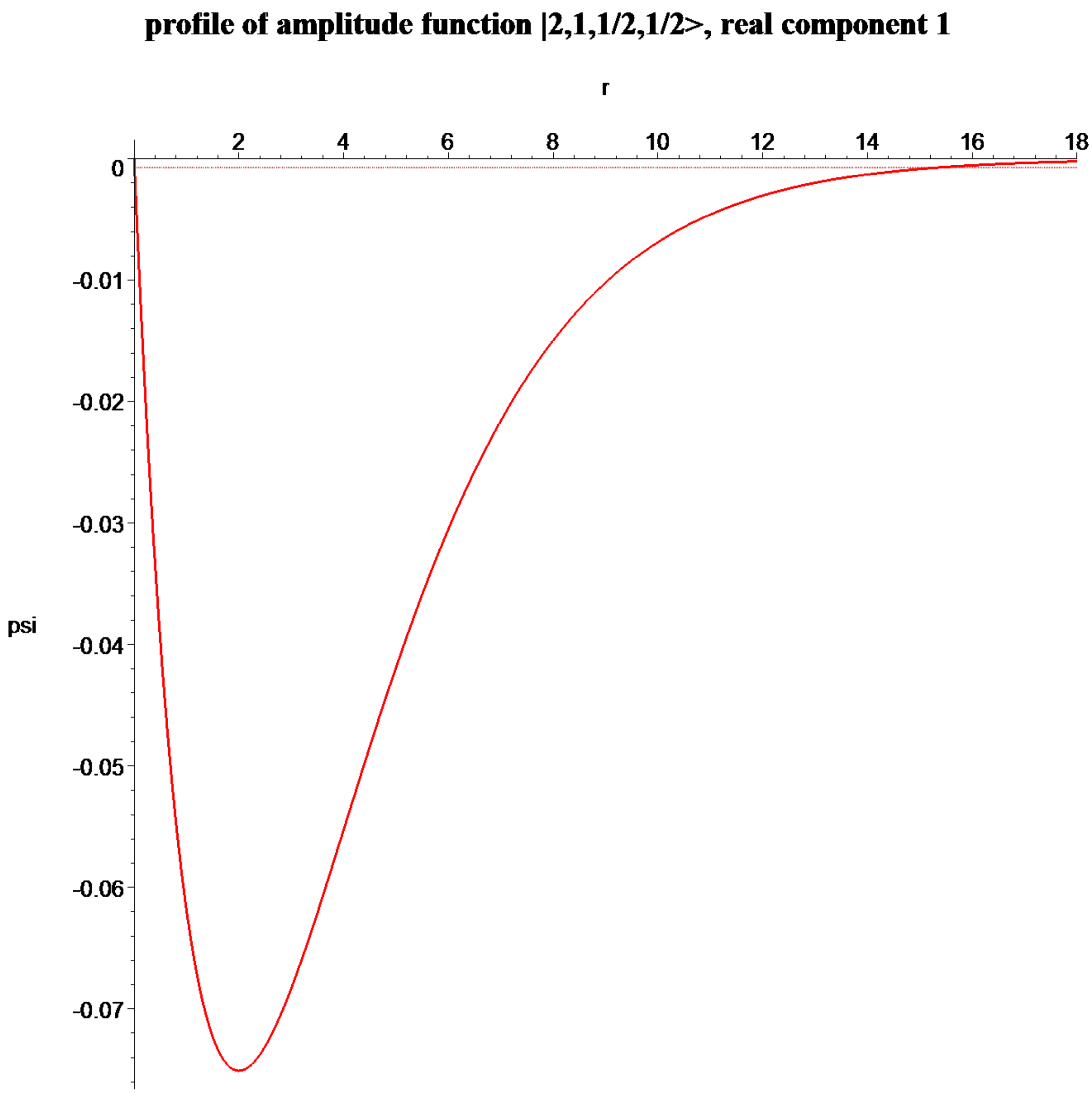
We investigate |2,1,1/2,1/2> analogously.

```
> '`|2,1,1/2,1/2>`' = `|2,1,1/2,1/2>`;
```

$$|2,1,1/2,1/2> = \begin{bmatrix} -\frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \cos(\theta) \\ -\frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\, \mathbf{e}^{(\phi I)} \\ \frac{1}{16} I \sqrt{2}\sqrt{3}\, \alpha\, Z \left(1 - \frac{r}{6}\right) \mathbf{e}^{\left(-\frac{r}{2}\right)} \\ 0 \end{bmatrix}$$

We plot the radial profile of the first component of |2,1,1/2,1/2> , which is purely real.

```
> plot([eval(`|2,1,1/2,1/2>`[1], theta=0), -0.00075], r=0..18,
    title="profile of amplitude function |2,1,1/2,1/2>, real
  component 1",
    titlefont=[TIMES,BOLD,14], colour=[red, brown, brown],
  linestyle=[1,2,2],
    labels=["r", "psi"], thickness=[3,2,2]);
```



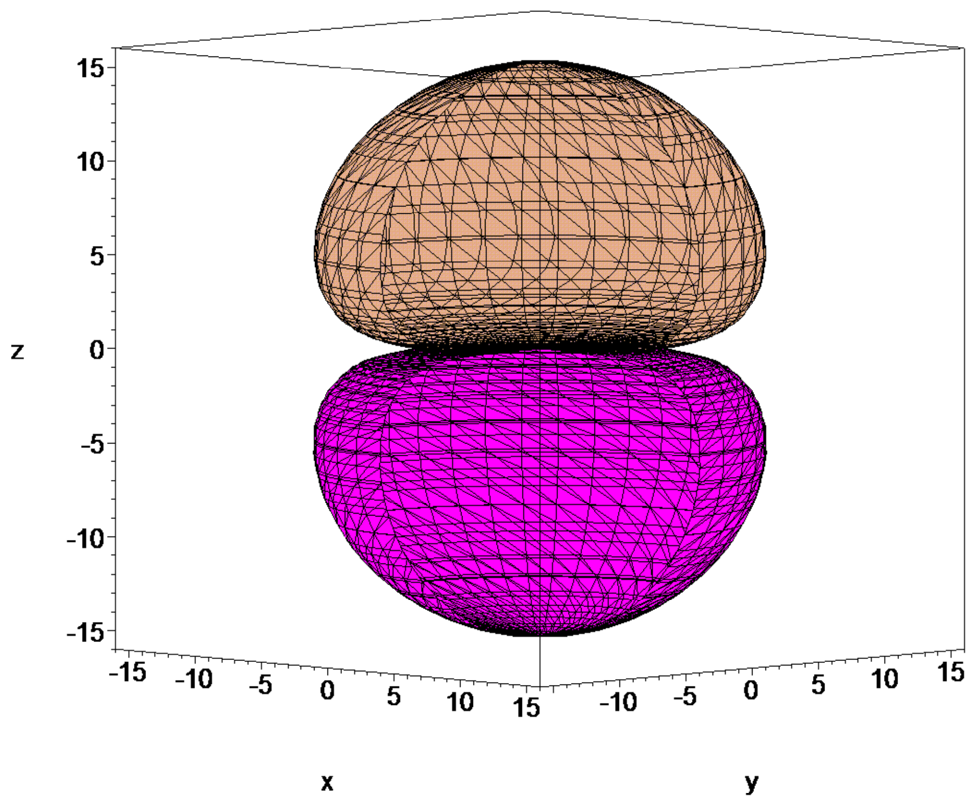
>

We plot the surface of this first component of |2,1,1/2,1/2> at a value of ψ that is $\frac{1}{100}$ of its maximum magnitude, cut open to show the lack of an inner lobe,

```
> plots[implicitplot3d]([`|2,1,1/2,1/2>`[1]=0.00075,
  `|2,1,1/2,1/2>`[1]=-0.00075],
     r=0..18, theta=0..Pi, phi=0..3/2*Pi, colour=[magenta, tan],
  labels=["x","y","z"],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |2,1,1/2,1/2>, real component 1",
  orientation=[-45,85],
```

```
titlefont=[TIMES,BOLD,14], view=[-16..16,-16..16,-16..16]);
```

amplitude function |2,1,1/2,1/2>, real component 1



>

which generates two separate nearly hemispherical lobes with rounded edges because of the angular dependence of this component; the overall shape is still roughly spherical and this surface resembles that of $\psi_{0,1,0}(r, \theta, \phi)$. The second component of |2,1,1/2,1/2> has real and imaginary parts;

```
> '`|2,1,1/2,1/2>`'[2] = evalc(`|2,1,1/2,1/2>`[2]);
```

$$|2,1,1/2,1/2>_2 = -\frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\phi) - \frac{1}{24} I \sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\sin(\phi)$$

```
> rp := Re(`|2,1,1/2,1/2>`[2]) assuming real;
```

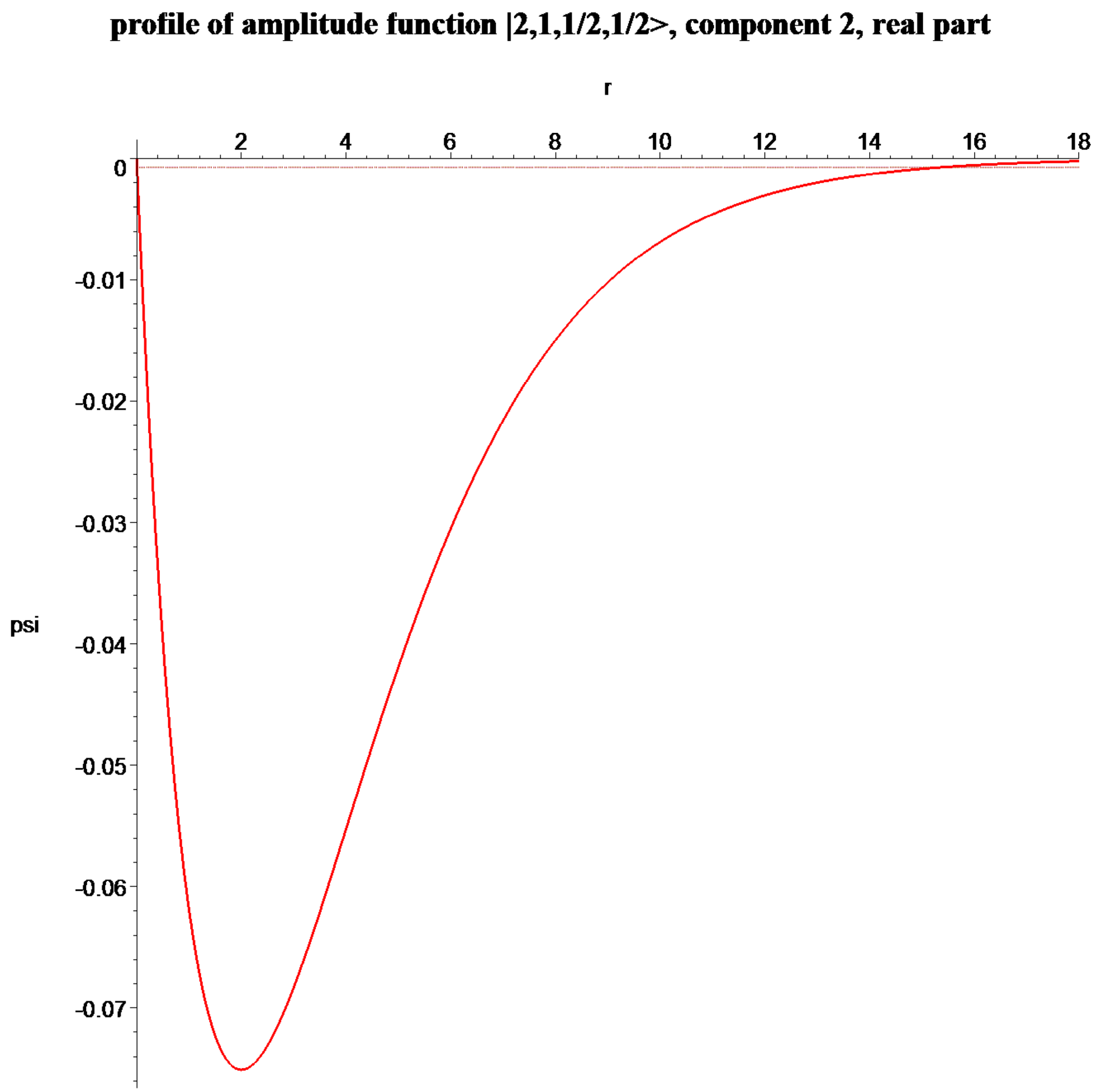
$$rp := -\frac{1}{24}\sqrt{2}\,\sqrt{3}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\phi)$$

```
> ip := Im(`|2,1,1/2,1/2>`[2]) assuming real;
```

$$ip := -\frac{1}{24}\sqrt{2}\,\sqrt{3}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\sin(\phi)$$

we plot first the profile of the real part along the polar axis, for which $\theta = 0$, to obtain the criterion for the surface,

```
> plot([eval(rp, [theta=Pi/2,phi=0,op(cond)]), -0.00075], 
  r=0..18,
      titlefont=[TIMES,BOLD,14], colour=[red, brown, brown],
      title="profile of amplitude function |2,1,1/2,1/2>, 
  component 2, real part",
      linestyle=[1,2,2], labels=["r", "psi"], thickness=[3,2]);
```

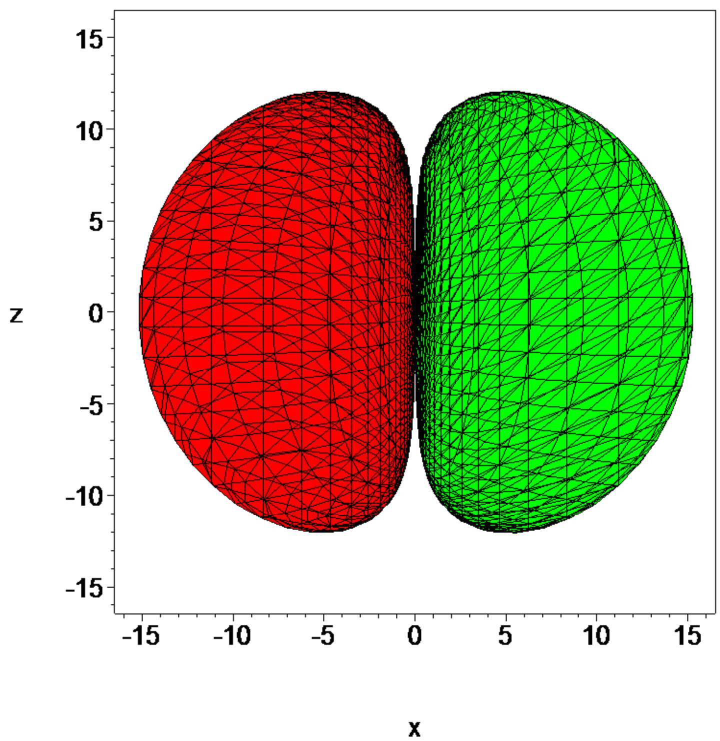



```
>
```

and then the surface itself.

```
> plots[implicitplot3d]([eval(rp, cond)=0.00075, eval(rp,
  cond)=-0.00075],
     r=0..17, theta=0..Pi, phi=0..2*Pi, colour=[red, green],
  orientation=[-90,90],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     labels=["x","y","z"], title="amplitude function
  |2,1,1/2,1/2>, component 2, real part",
     titlefont=[TIMES,BOLD,14],
  view=[-16.5..16.5,-16.5..16.5,-16.5..16.5]);
```

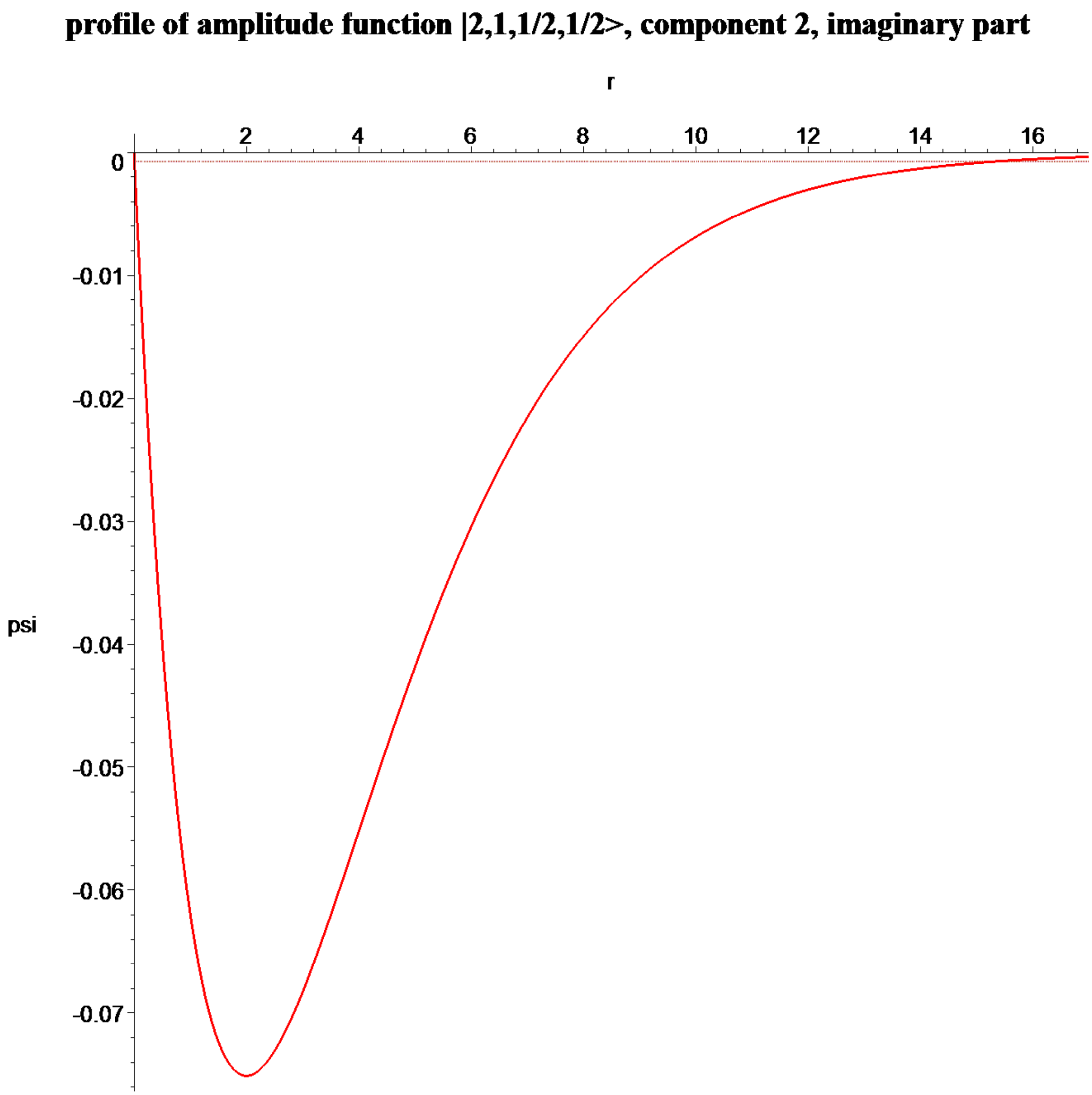
amplitude function |2,1,1/2,1/2>, component 2, real part



>

we plot next the profile of the imaginary part along the polar axis, for which θ = 0, to obtain the criterion for the surface,

```
> plot([eval(ip, [theta=Pi/2,phi=Pi/2,op(cond)]), -0.00075],
      r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,1/2,1/2>,
  component 2, imaginary part",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

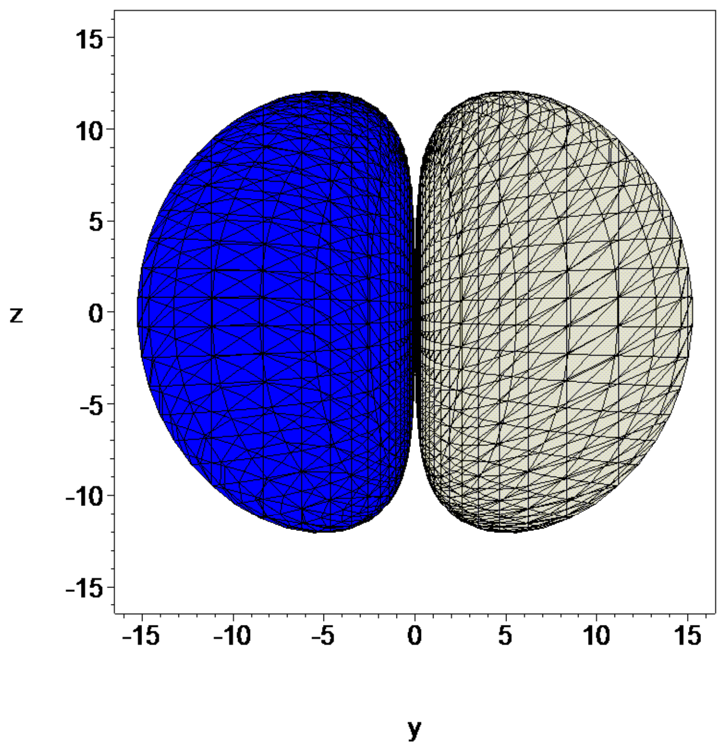



```
>
```

and then the surface itself.

```
> plots[implicitplot3d]([eval(ip, cond)=0.00075, eval(ip,
  cond)=-0.00075],
     r=0..17, theta=0..Pi, phi=0..2*Pi, colour=[blue, wheat],
  orientation=[0,90],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     labels=["x","y","z"], title="amplitude function
  |2,1,1/2,1/2>, component 2, imaginary part",
     titlefont=[TIMES,BOLD,14],
  view=[-16.5..16.5,-16.5..16.5,-16.5..16.5]);
```

amplitude function |2,1,1/2,1/2>, component 2, imaginary part



>

The latter two surfaces resemble those of the corresponding real and imaginary parts of $\psi_{0,1,-1}(r, \theta, \phi)$. Whereas the fourth component is identically zero, the third component,

```
> '`|2,1,1/2,1/2>`'[3] = expand(`|2,1,1/2,1/2>`[3]);
```

$$|2,1,1/2,1/2>_3 = \frac{1}{16} I \sqrt{2}\sqrt{3}\,\alpha Z \mathbf{e}^{\left(-\frac{r}{2}\right)} - \frac{1}{96} I \sqrt{2}\sqrt{3}\,\alpha Z \mathbf{e}^{\left(-\frac{r}{2}\right)} r$$

```
> op1 := simplify(Im(op(1,expand(`|2,1,1/2,1/2>`[3])))) assuming
  real;
```

$$op1 := \frac{1}{16}\sqrt{2}\sqrt{3}\,\alpha Z \mathbf{e}^{\left(-\frac{r}{2}\right)}$$

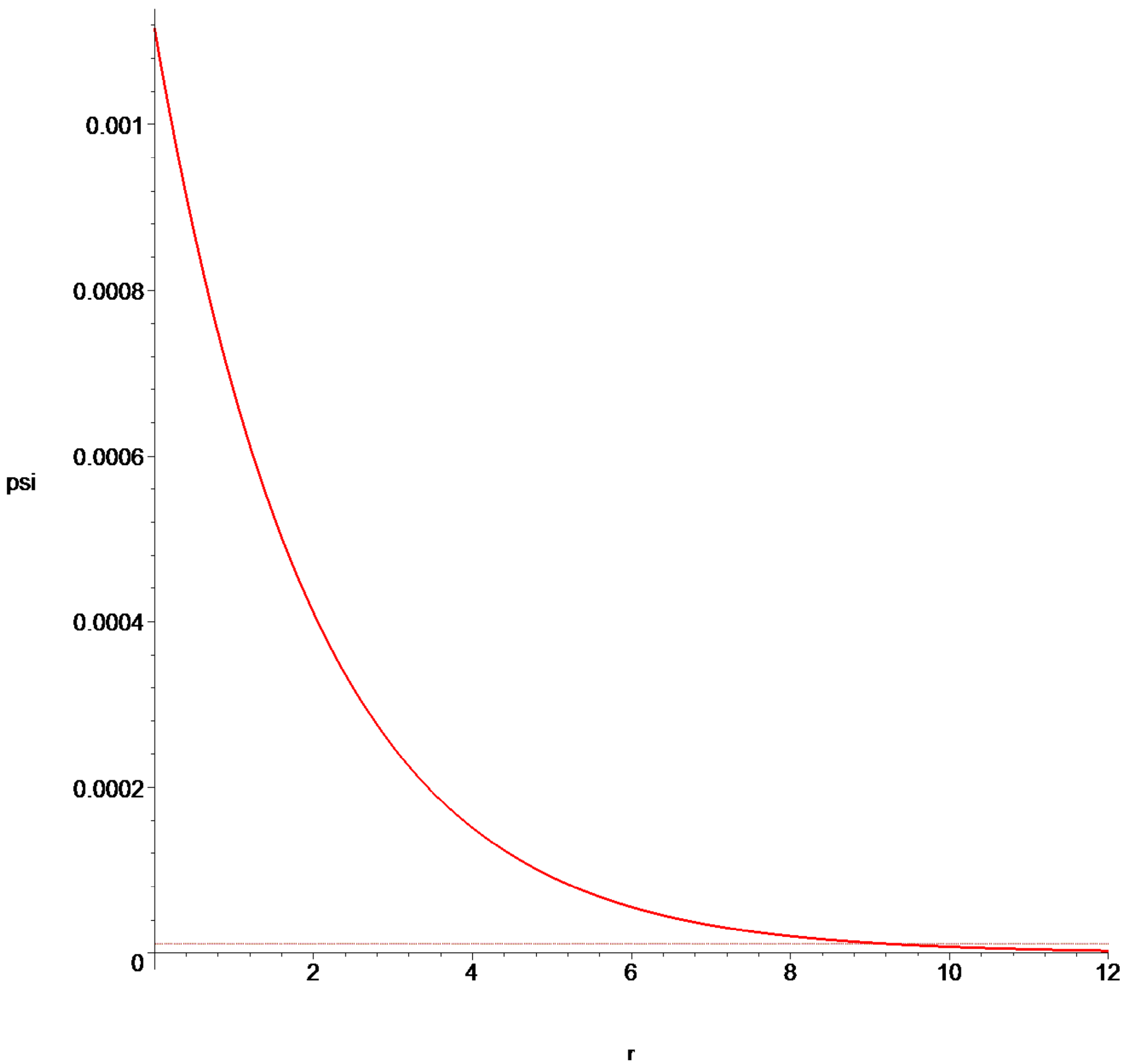
```
> op2 := simplify(Im(op(2,expand(`|2,1,1/2,1/2>`[3])))) assuming
  real;
```

$$op2 := -\frac{1}{96}\sqrt{2}\,\sqrt{3}\,\alpha\,Z\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\,r$$

which we split into two parts, is purely imaginary and lacks an angular dependence; the first part has this profile that we apply to obtain the criterion for the surface.

```
> plot([eval(op1, cond), 0.0000115], r=0..12,
  titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,1/2,1/2>,
  imaginary component 3, inner part",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

profile of amplitude function |2,1,1/2,1/2>, imaginary component 3, inner part

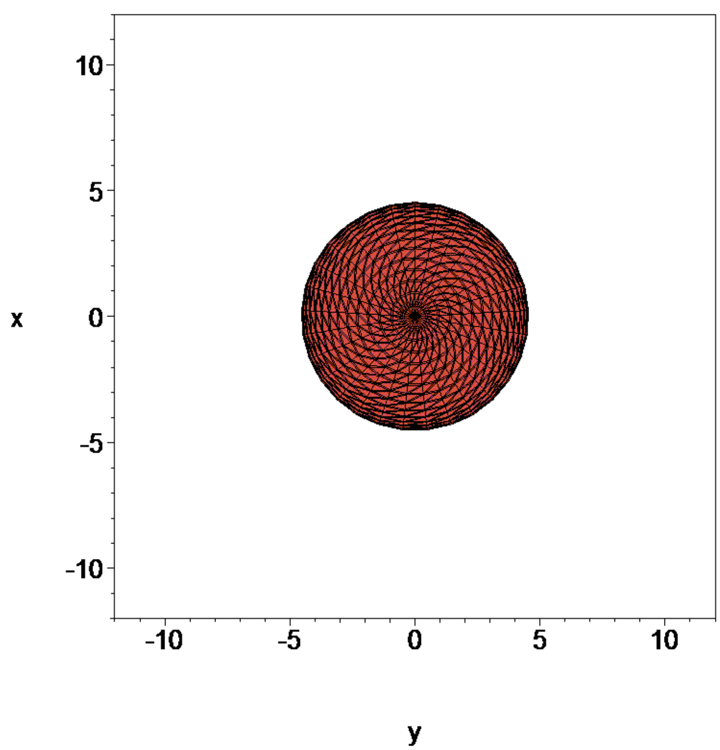


>

We plot the surface itself in its imaginary part to show the inner lobe.

```
> pl1 := plots[implicitplot3d](eval(op1, cond)=1.15e-4, r=0..7,
  theta=0..Pi,
     phi=0..2*Pi, colour=orange, orientation=[0,180],
  labels=["x","y","z"],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |2,1,1/2,1/2>, imaginary component
  3, inner part",
     titlefont=[TIMES,BOLD,14], view=[-12..12,-12..12,-12..12]):
  pl1;
```

amplitude function |2,1,1/2,1/2>, imaginary component 3, inner part

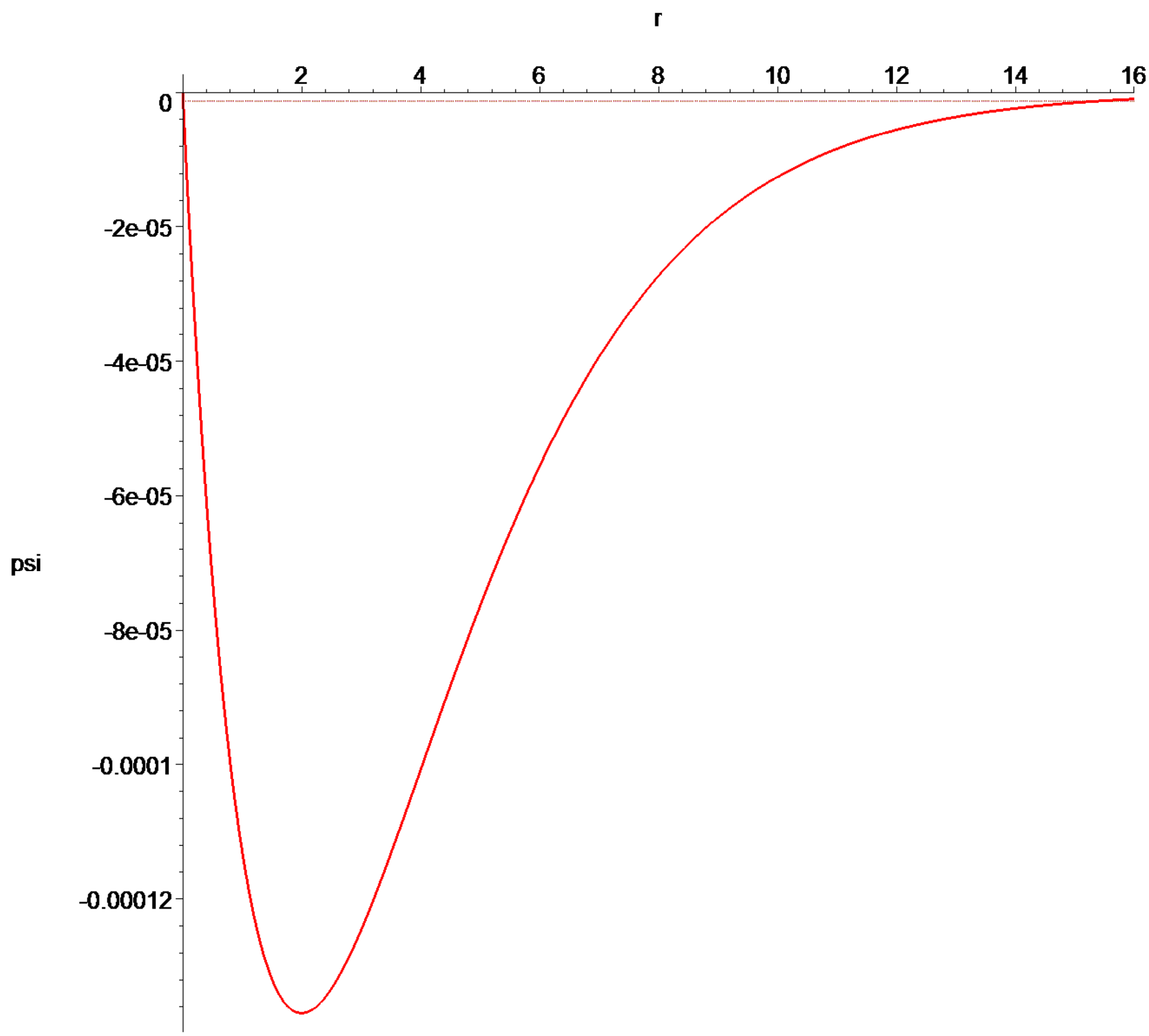


>

We plot the radial profile of the other part of imaginary component 3 of amplitude function |2,1,1/2,1/2>,

```
> plot([eval(op2, cond), -1.36e-6], r=0..16,
  titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,1/2,1/2>,
  imaginary component 3, outer part",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

profile of amplitude function |2,1,1/2,1/2>, imaginary component 3, outer part



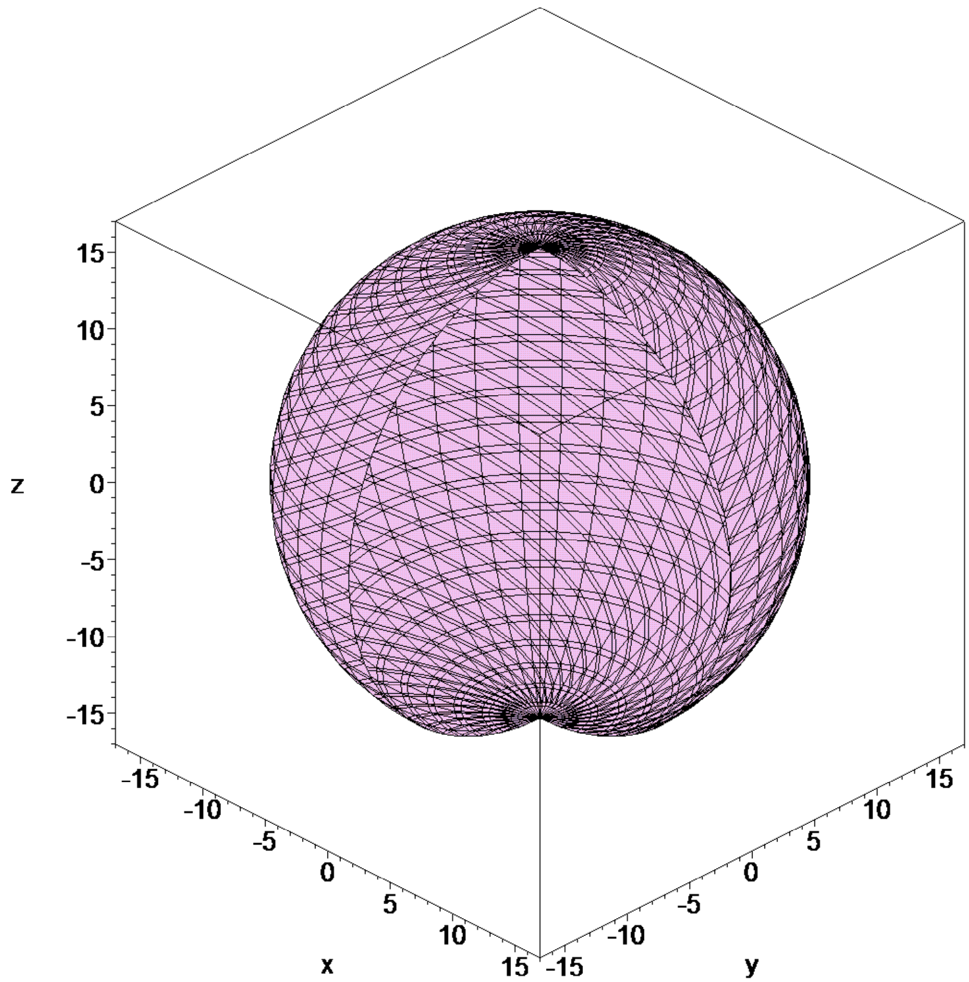
>

which yields this surface, cut open to show the lack of internal strucutre.

```
> pl2 := plots[implicitplot3d](eval(op2, cond)=-1.36e-6, r=0..16,
  theta=0..Pi,
```

```
   phi=0..3/2*Pi, colour=plum, orientation=[-45,60],
labels=["x","y","z"],
   coords = scispherical, grid=[30,30,30], scaling=constrained,
axes=box,
   title="amplitude function |2,1,1/2,1/2>, imaginary component
3",
   titlefont=[TIMES,BOLD,14], view=[-17..17,-17..17,-17..17]):
pl2;
```

amplitude function |2,1,1/2,1/2>, imaginary component 3

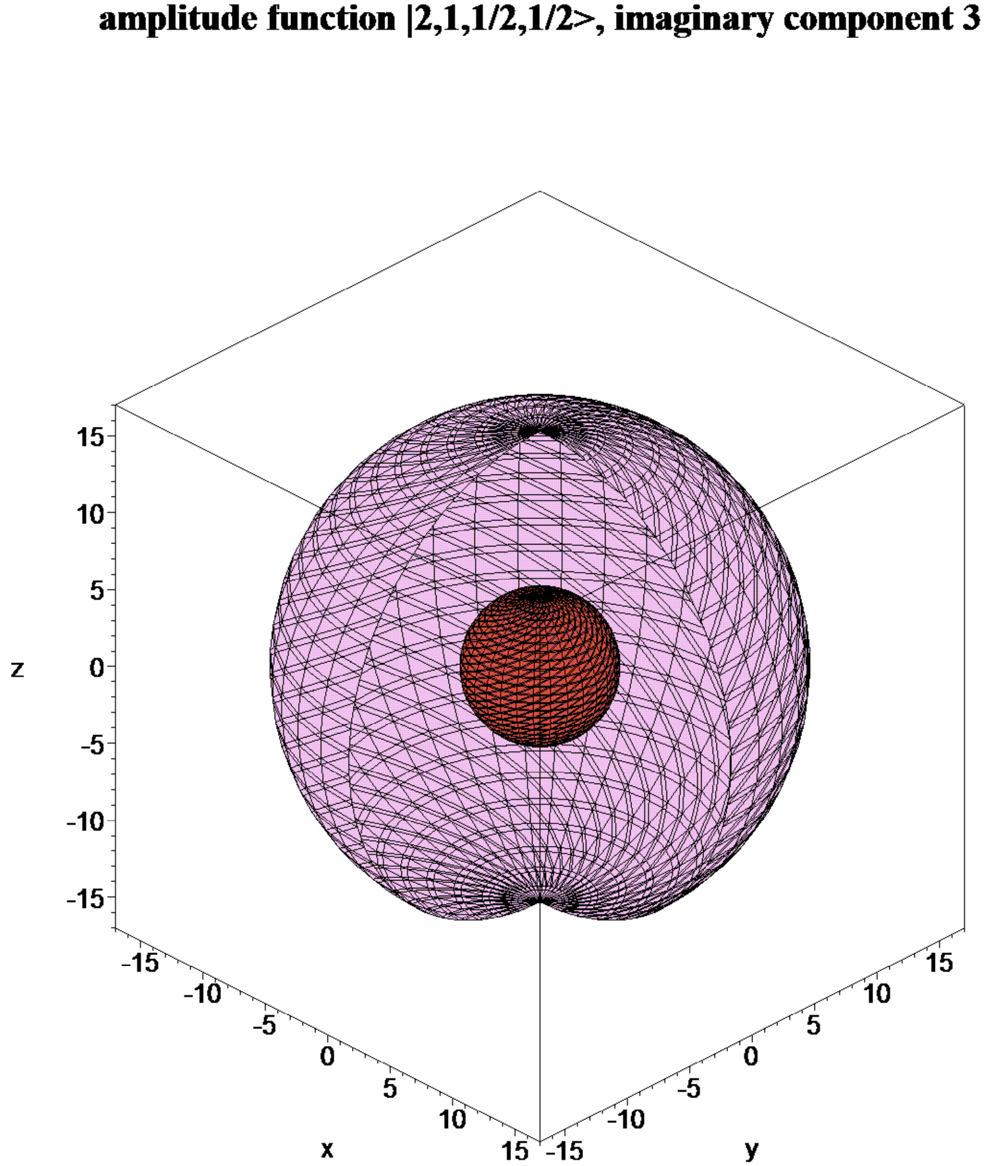


\>

We combine these two plots to produce surfaces of the inner lobe and the outer lobe.

```
> plots[display](pl1,pl2, orientation=[-45,60],
  titlefont=[TIMES,BOLD,14],
```

```
   title="amplitude function |2,1,1/2,1/2>, imaginary component
3",
   view=[-17..17,-17..17,-17..17]);
```



>

This imaginary surface resembles that of real function $\psi_{1,0,0}(r, \theta, \phi)$. From |2,1,1/2,1/2>,

```
> p := evalc(`|2,1,1/2,1/2>`);
```

$$p := \begin{bmatrix} -\frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \cos(\theta) \\ -\frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\phi) - \frac{1}{24} I \sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\sin(\phi) \\ \frac{1}{16} I \sqrt{2}\sqrt{3}\, \alpha Z \left(1 - \frac{r}{6}\right) \mathbf{e}^{\left(-\frac{r}{2}\right)} \\ 0 \end{bmatrix}$$

and its complex conjugate,

```
> pc := evalc(subs(I=-I,`|2,1,1/2,1/2>`));
```

$$pc := \begin{bmatrix} -\frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \cos(\theta) \\ -\frac{1}{24}\sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\phi) + \frac{1}{24} I \sqrt{2}\sqrt{3}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\sin(\phi) \\ \frac{-1}{16} I \sqrt{2}\sqrt{3}\, \alpha Z \left(1 - \frac{r}{6}\right) \mathbf{e}^{\left(-\frac{r}{2}\right)} \\ 0 \end{bmatrix}$$

we form scalar product |2,1,1/2,1/2>* **.** |2,1,1/2,1/2>,

```
> ps :=
  simplify(evalc(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,1/2,1/2
  >`)) . `|2,1,1/2,1/2>`)) assuming real;
```

$$ps := \frac{1}{1536} \mathbf{e}^{(-r)} (Z^2 \alpha^2 r^2 - 12 Z^2 \alpha^2 r + 36 Z^2 \alpha^2 + 16 r^2)$$

We separate the terms according to their content.

```
> fl := simplify(remove(has, expand(ps), alpha));
```

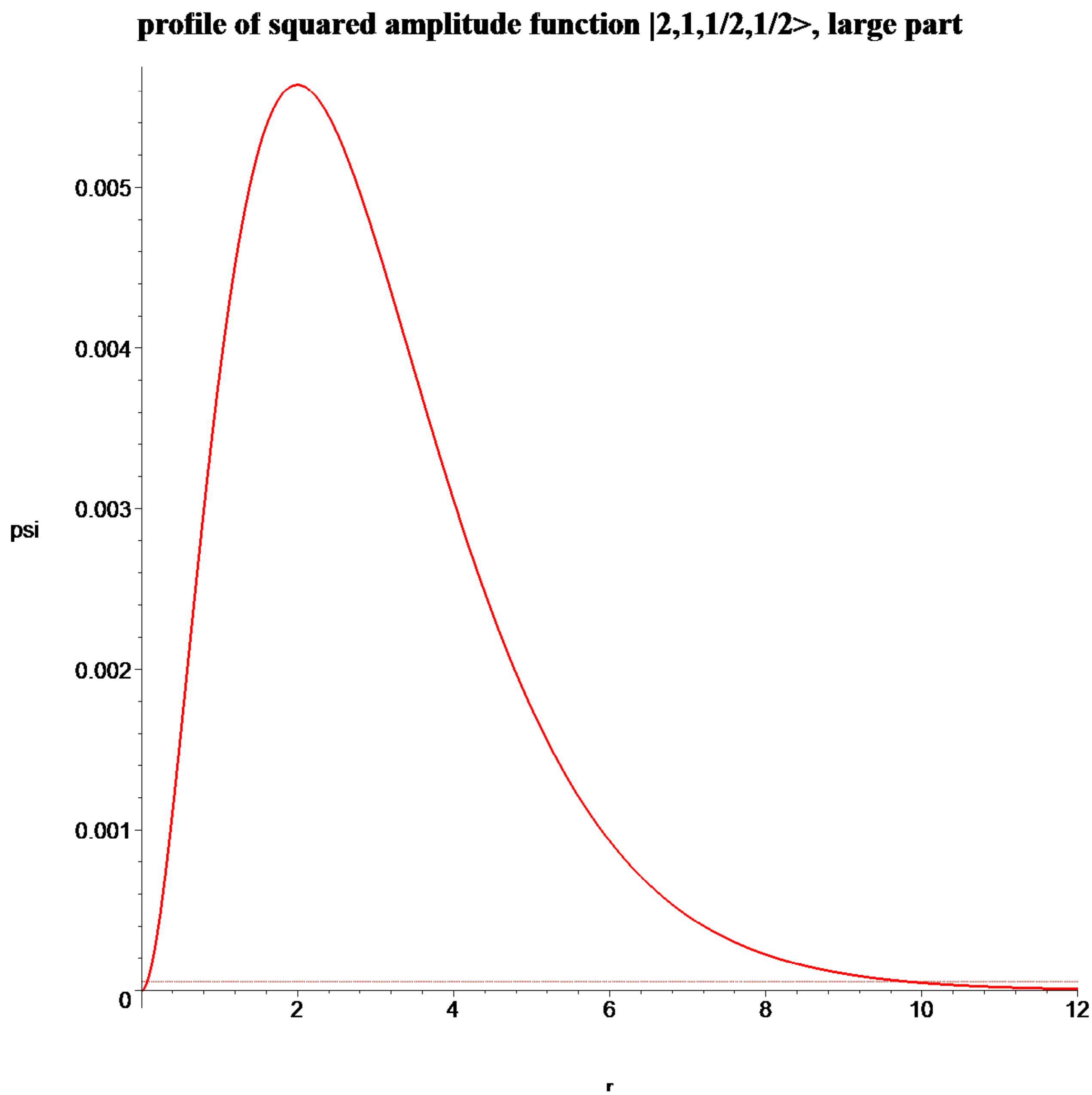
$$fl := \frac{1}{96} \mathbf{e}^{(-r)} r^2$$

```
> fs := simplify(ps - fl);
```

$$fs := \frac{1}{1536} \mathbf{e}^{(-r)} Z^2 \alpha^2 (r - 6)^2$$

and plot the radial profile of the large part.

```
> plot([eval(fl, cond), 0.000053], r=0..12, linestyle=[1,2],
        title="profile of squared amplitude function
  |2,1,1/2,1/2>, large part",
        titlefont=[TIMES,BOLD,14], colour=[red, brown],
        labels=["r", "psi"], thickness=[3,2]);
```

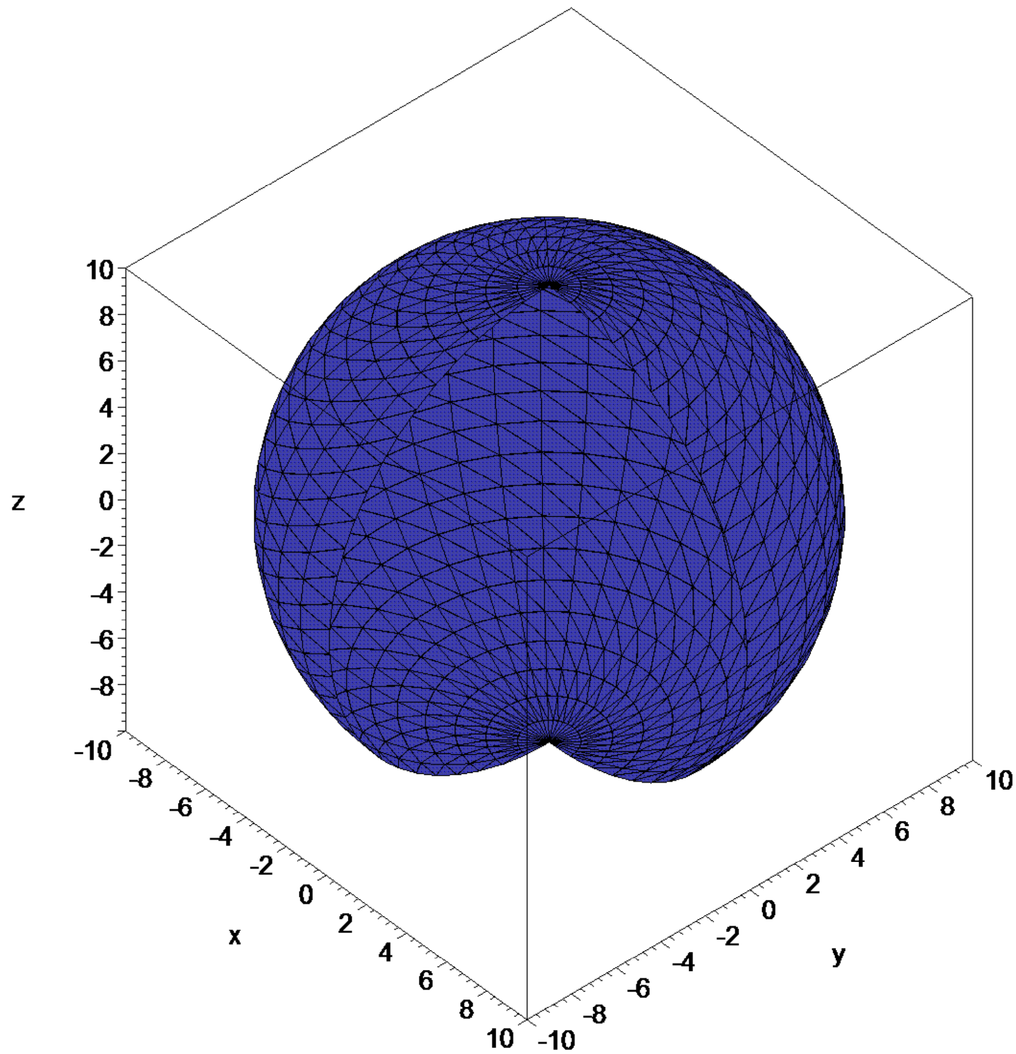



```
>
```

For that large part of |2,1,1/2,1/2> squared we plot its surface, cut open,

```
> plots[implicitplot3d](eval(fl, cond)=0.000053, r=0..11,
  theta=0..Pi, phi=0..3/2*Pi,
     colour=navy, orientation=[-42,50],
     labels=["x","y","z"], coords = scispherical,
  grid=[30,30,30], axes=box,
     title="squared amplitude function |2,1,1/2,11/2>, large
  part",
     scaling=constrained, titlefont=[TIMES,BOLD,14],
  view=[-10..10,-10..10,-10..10]);
```

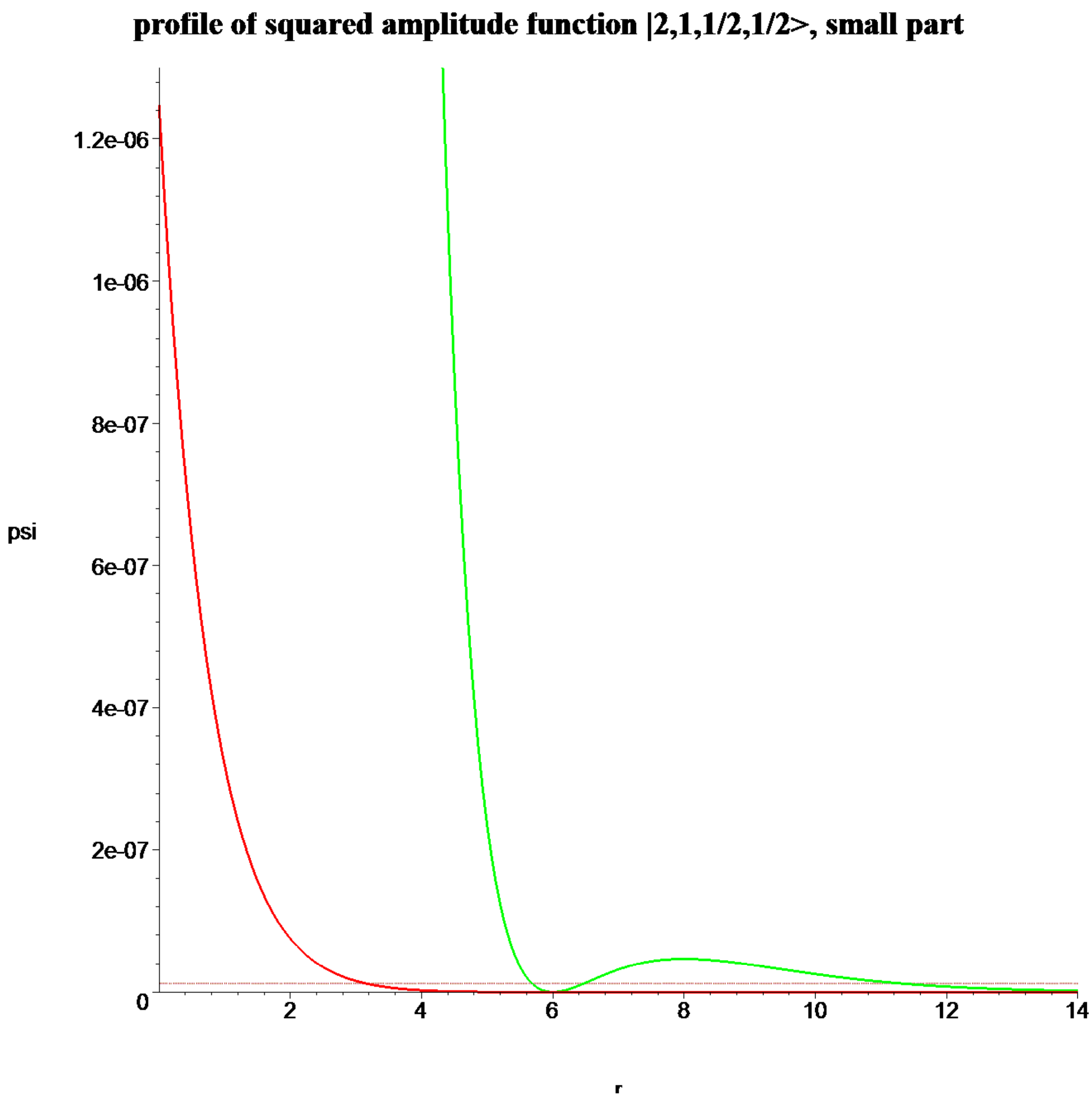
squared amplitude function |2,1,1/2,11/2>, large part




```
>
```

which yields one spherical lobe. The small component has a radial profile according to the red curve; the maginfication times 1000 in the green curve shows a node r = 6 units and a local maximum about r = 8 units.

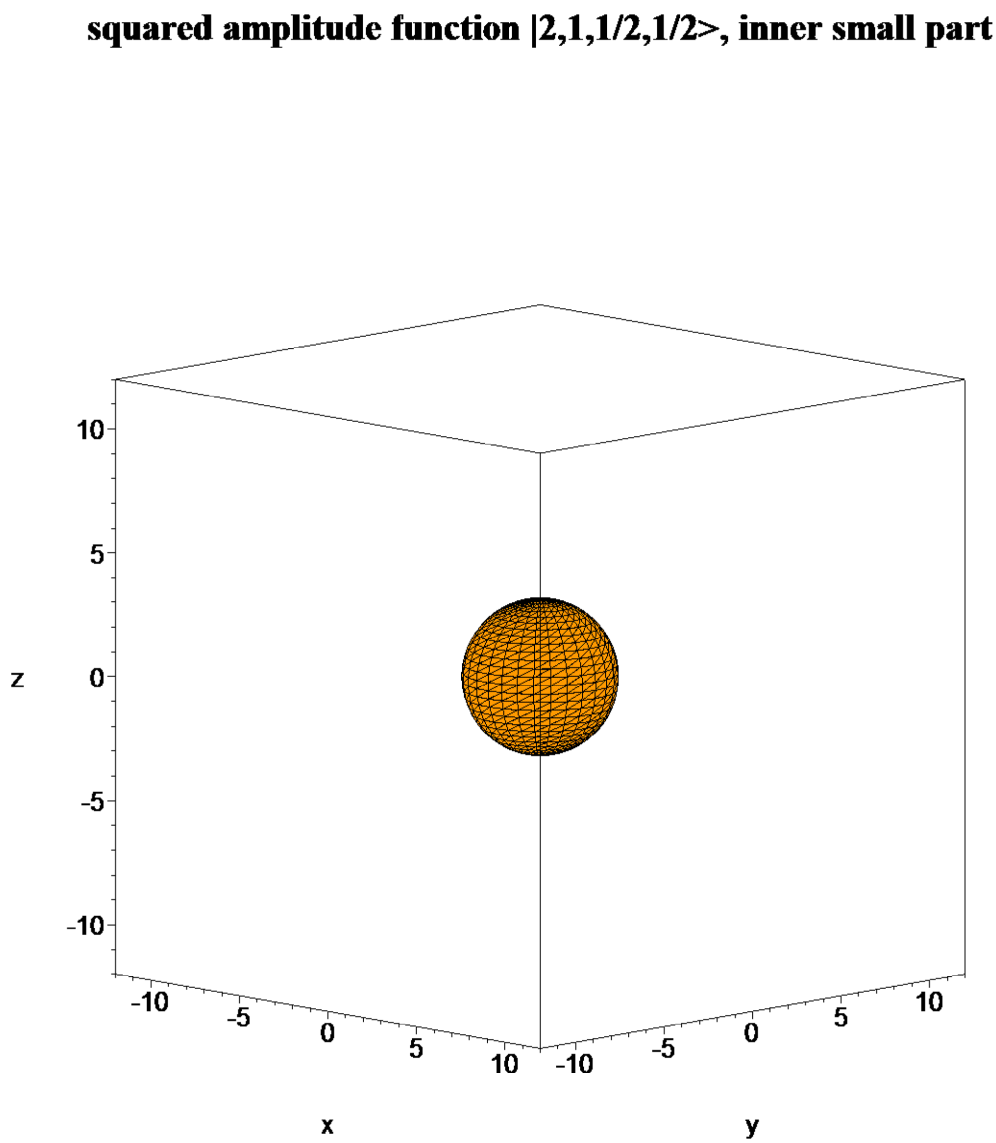
```
> plot([eval(fs, cond), 1000*eval(fs, cond), 1.24e-8], r=0..14,
  0..1.3e-6,
     title="profile of squared amplitude function |2,1,1/2,1/2>,
  small part",
     titlefont=[TIMES,BOLD,14], colour=[red, green, brown],
  linestyle=[1,1,2],
     labels=["r", "psi"], thickness=[3,3,2]);
```




```
>
```

We accordingly plot the surface of the large part of |2,1,1/2,1/2> squared, showing first the inner surface at the standard criterion of ψ,

```
> pl1 := plots[implicitplot3d](eval(fs, cond)=1.24e-8,
     r=0..13, theta=0..Pi, phi=0..2*Pi, colour=coral,
  labels=["x","y","z"],
     orientation=[-45,80],coords = scispherical, grid=[30,30,30],
  scaling=constrained,
     axes=box, title="squared amplitude function |2,1,1/2,1/2>,
  inner small part",
     titlefont=[TIMES,BOLD,14], view=[-12..12,-12..12,-12..12]):
  pl1;
```



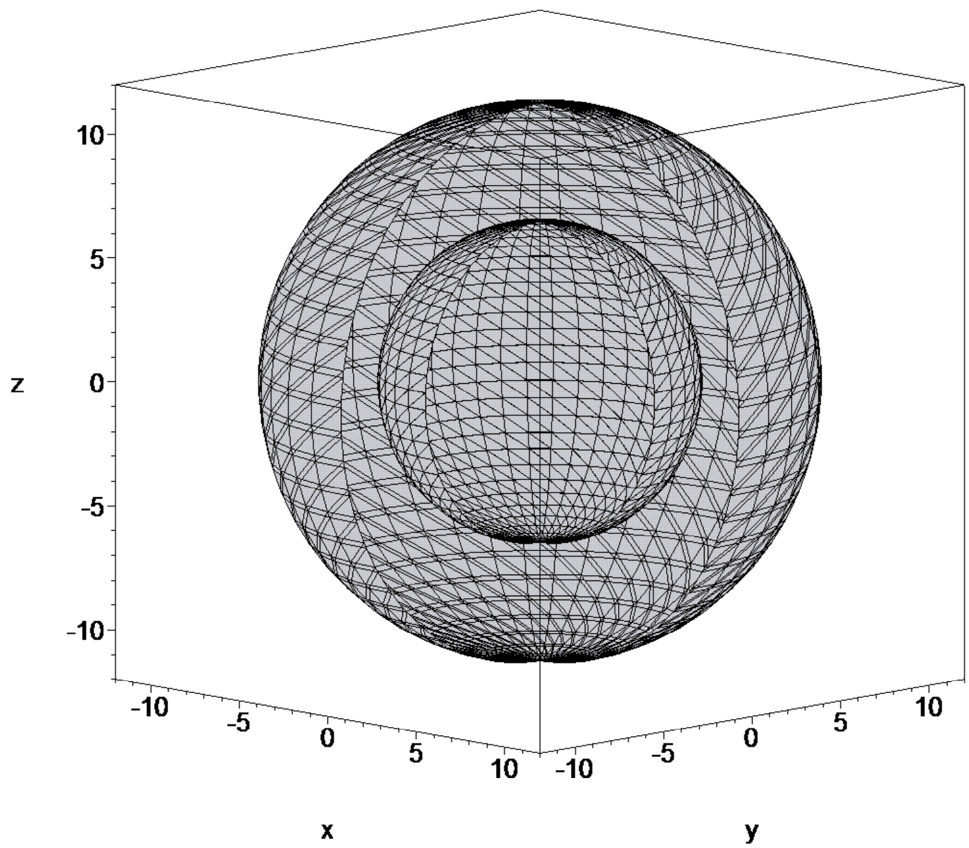

```
>
```

which shows only a spherical inner lobe; when we decrease the criterion for the surface to be less than the secondary extremum near $r = 6$, we see the outer surface.

```
> pl2 := plots[implicitplot3d](eval(fs, cond)*1000=1.24e-8,
  r=6..13,
     theta=0..Pi, phi=0..3/2*Pi, colour=grey,
  labels=["x","y","z"],  axes=box,
     orientation=[-45,80],coords = scispherical, grid=[30,30,30],
  scaling=constrained,
     title="squared amplitude function |2,1,1/2,1/2>, amplified
  small part",
     titlefont=[TIMES,BOLD,14], view=[-12..12,-12..12,-12..12]):
```

```
pl2;
```

squared amplitude function |2,1,1/2,1/2>, amplified small part

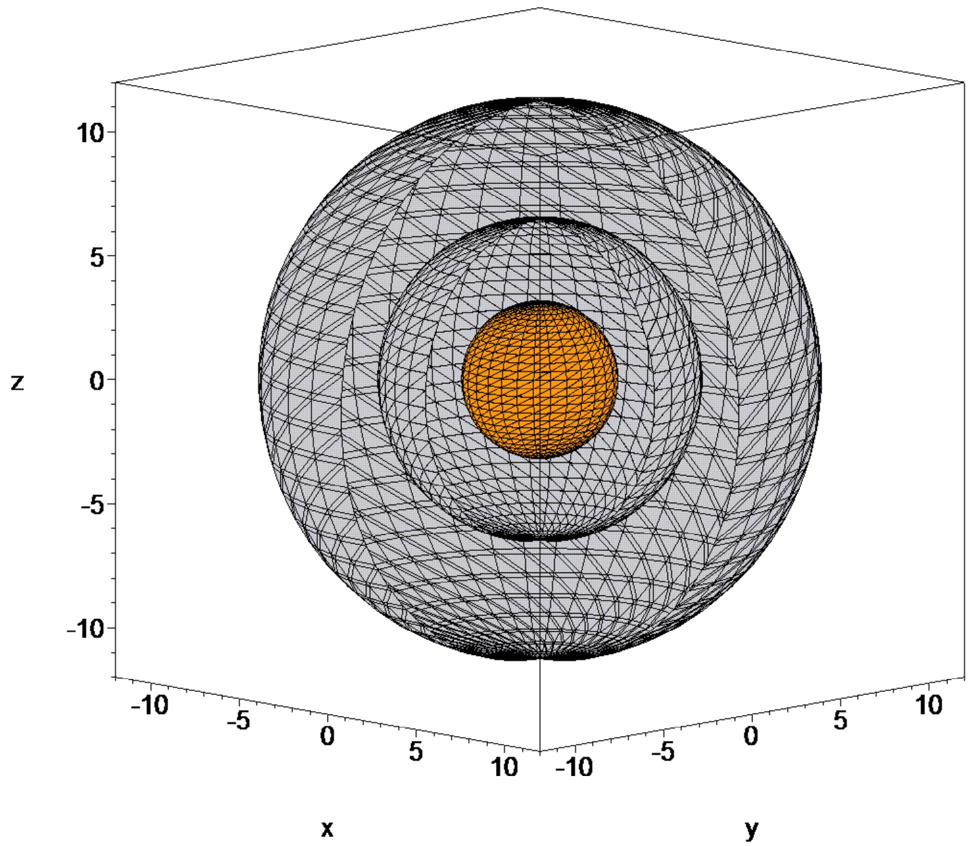



```
>
```

We plot the two parts together.

```
> plots[display](pl1,pl2, titlefont=[TIMES,BOLD,14],
      title="squared amplitude function |2,1,1/2,1/2>, both
  parts");
```

squared amplitude function |2,1,1/2,1/2>, both parts



>

This surface of the small part resembles that of $\psi_{1,\,0,\,0}(r,\,\theta,\,\phi)$, whereas the surface of the large part has no counterpart as a direct solution of Schroedinger's equation for the hydrogen atom.

We proceed to investigate |2,1,3/2,3/2>.

```
> '`|2,1,3/2,3/2>`' = `|2,1,3/2,3/2>`;
```

$$|2,1,3/2,3/2\rangle = \begin{bmatrix} \frac{1}{8} r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\, \mathbf{e}^{(\phi I)} \\ 0 \\ \frac{1}{32} I \alpha Z r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta) \cos(\theta)\, \mathbf{e}^{(\phi I)} \\ \frac{1}{32} I \alpha Z r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2\, \mathbf{e}^{(2 I \phi)} \end{bmatrix}$$

For the first component of |2,1,3/2,3/2>, which is complex,

```
> '`|2,1,3/2,3/2>`'[1] = evalc(`|2,1,3/2,3/2>`[1]) assuming real;
```

$$|2,1,3/2,3/2\rangle_1 = \frac{1}{8} r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta) \cos(\phi) + \frac{1}{8} I r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta) \sin(\phi)$$

```
> rp := Re(`|2,1,3/2,3/2>`[1]) assuming real;
```

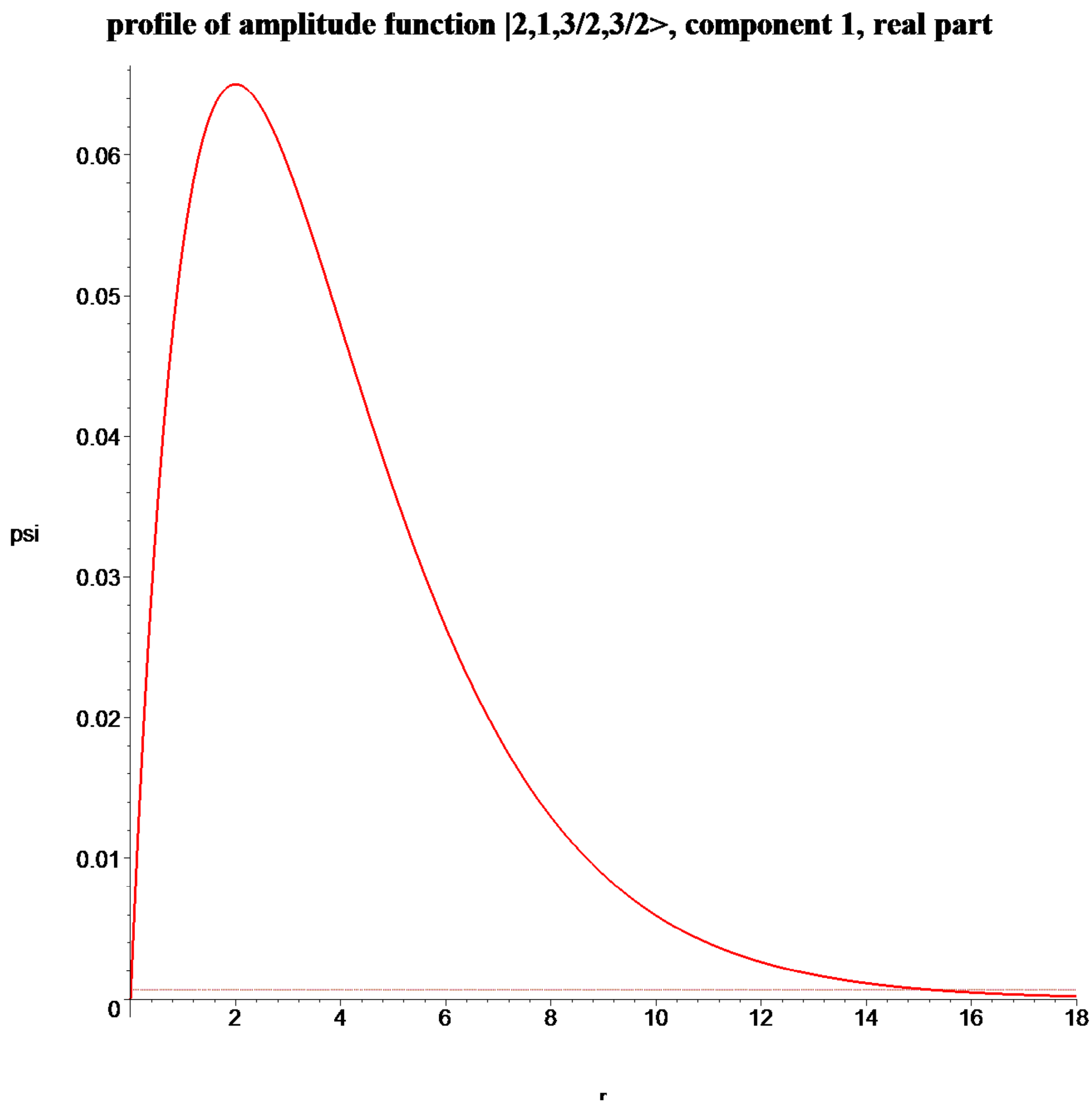
$$rp := \frac{1}{8} r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta) \cos(\phi)$$

```
> ip := Im(`|2,1,3/2,3/2>`[1]) assuming real;
```

$$ip := \frac{1}{8} r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta) \sin(\phi)$$

we plot the radial profile of the real part.

```
> plot([eval(ip, [theta=Pi/2, phi=Pi/4]), 0.00066], r=0..18,
    title="profile of amplitude function |2,1,3/2,3/2>,
  component 1, real part",
    titlefont=[TIMES,BOLD,14], colour=[red, brown, brown],
  linestyle=[1,2],
    labels=["r", "psi"], thickness=[3,2]);
```



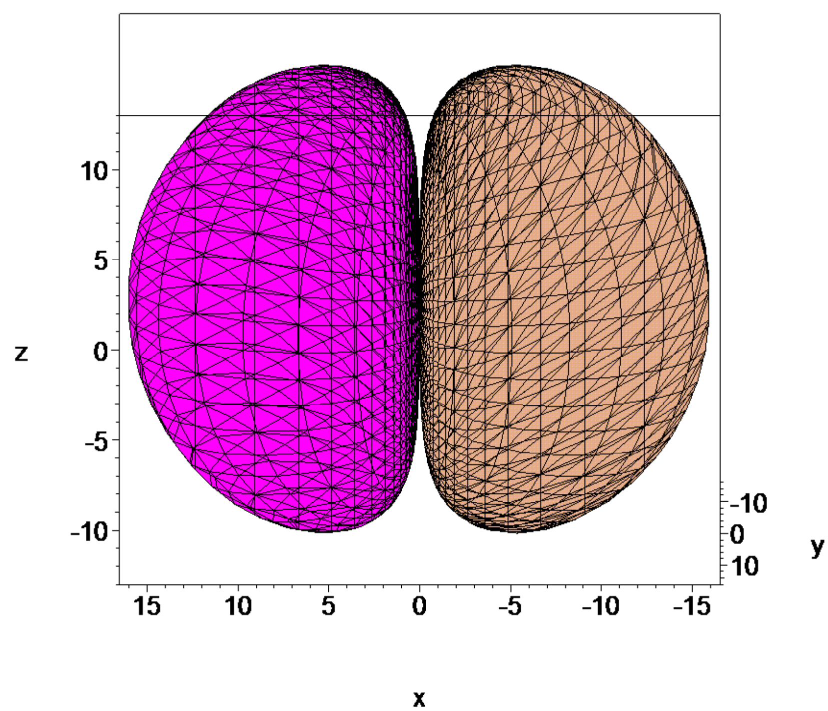
>

We plot the surface of the real part of this first component of |2,1,1/2,1/2> at a value of ψ that is $\frac{1}{100}$ of its maximum magnitude,

```
> plots[implicitplot3d]([rp=0.00066, rp=-0.00066], r=0..18,
  theta=0..Pi, phi=0..2*Pi,
     colour=[magenta, tan], labels=["x","y","z"],
  orientation=[90,80],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |2,1,1/2,1/2>, component 1, real
  part",
```

```
   titlefont=[TIMES,BOLD,14],
  view=[-16.5..16.5,-16..16,-13..13]);
```

amplitude function |2,1,1/2,1/2>, component 1, real part



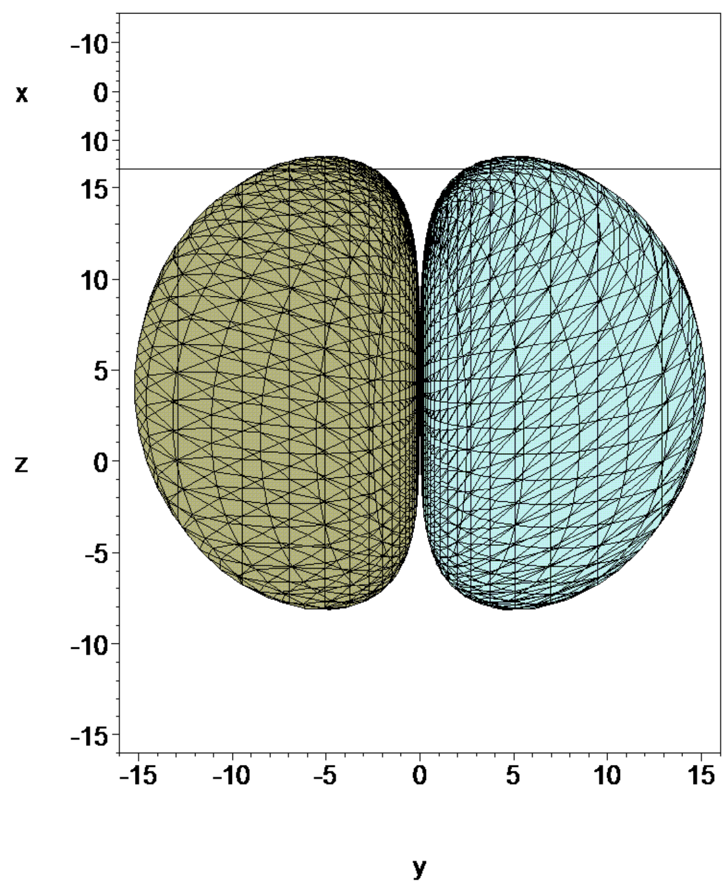
>

which generates two separate nearly hemispherical lobes because of the angular dependence of this component; the overall shape is still roughly spherical. We plot the corresponding imaginary part of the first component of |2,1,3/2,3/2>.

```
> plots[implicitplot3d]([ip=0.00094, ip=-0.00094], r=0..18,
  theta=0..Pi, phi=0..2*Pi,
     colour=[turquoise, khaki], labels=["x","y","z"],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |2,1,3/2,3/2>, component 1,
```

```
imaginary part",
   orientation=[0,75], titlefont=[TIMES,BOLD,14],
view=[-16..16,-16..16,-16..16]);
```

amplitude function |2,1,3/2,3/2>, component 1, imaginary part



\>

These two plots resemble those of the surfaces of $\psi_{0,\,1,\,-1}(r,\theta,\phi)$. The second component of |2,1,3/2,3/2> is zero but the third component has real and imaginary parts;

```
> '`|2,1,3/2,3/2>`'[3] = evalc(`|2,1,3/2,3/2>`[3]);
```

$|2,1,3/2,3/2>_3 =$

$$-\frac{1}{32}\alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\sin(\phi)+\frac{1}{32} I\,\alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\cos(\phi)$$

```
> rp := Re(`|2,1,3/2,3/2>`[3]) assuming real;
```

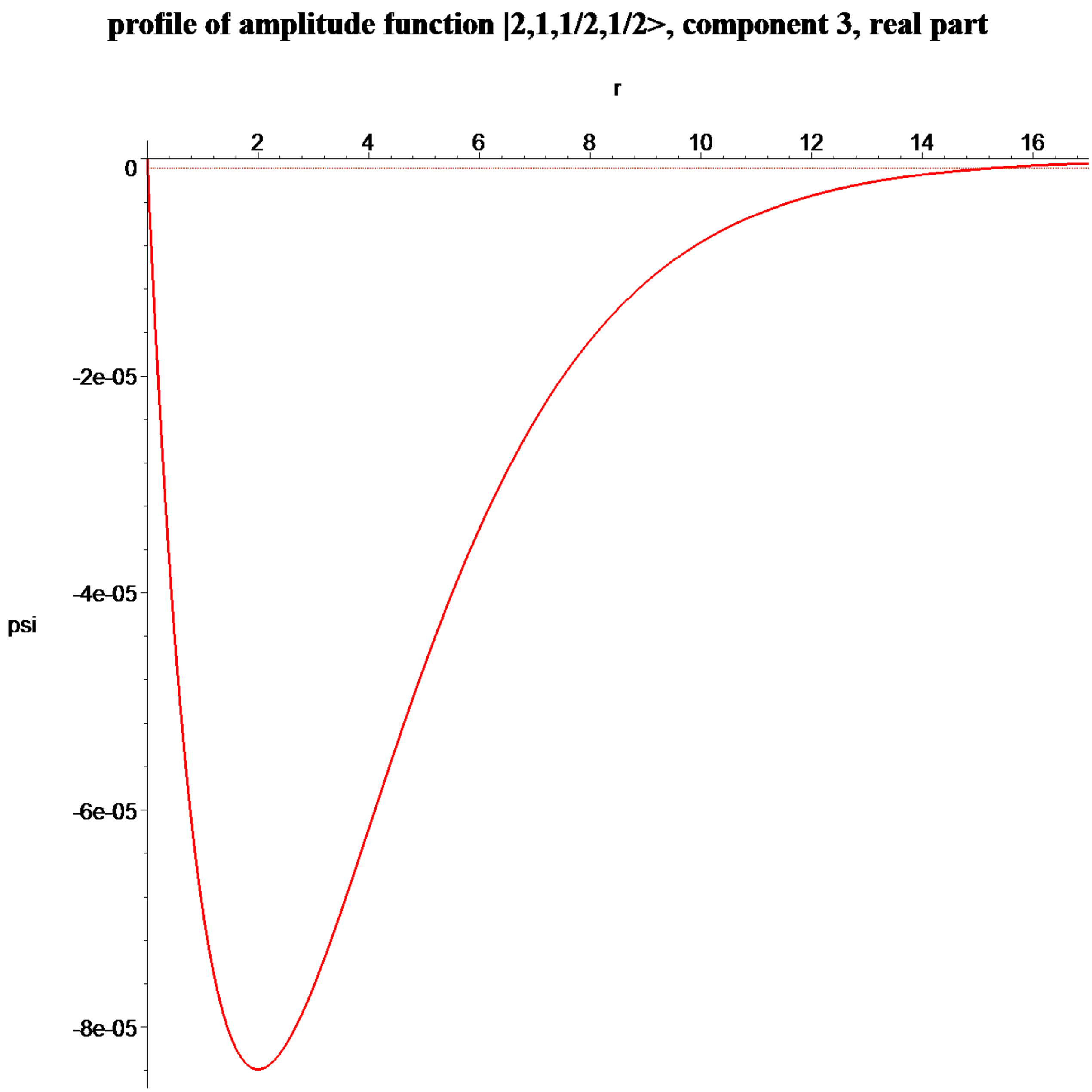
$$rp := -\frac{1}{32}\,\alpha\, Z\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\sin(\phi)$$

```
> ip := Im(`|2,1,3/2,3/2>`[3]) assuming real;
```

$$ip := \frac{1}{32}\,\alpha\, Z\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\cos(\phi)$$

we plot first the radial profile of the real part along the polar axis, for which $\theta = 0$, to obtain the criterion for the surface,

```
> plot([eval(rp, [theta=Pi/4,phi=Pi/2,op(cond)]), -8.4e-7],
      r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,1/2,1/2>,
  component 3, real part",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

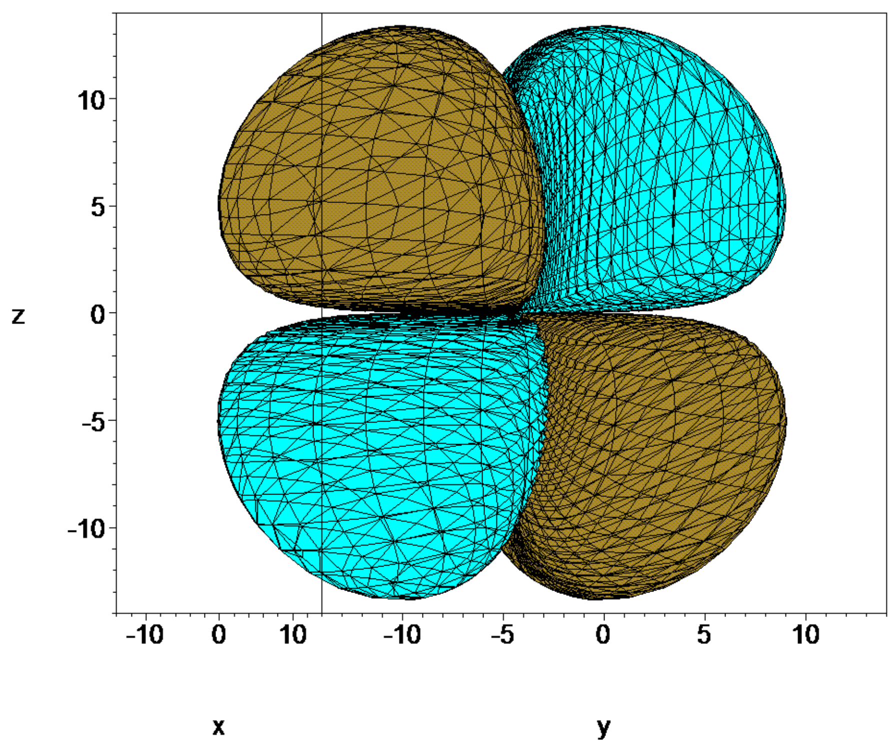


>

and then the surface itself.

```
> plots[implicitplot3d]([eval(rp, cond)=8.4e-7,  eval(rp,
  cond)=-8.4e-7],
     r=0..17, theta=0..Pi, phi=0..2*Pi, colour=[sienna, cyan],
  orientation=[-20,90],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     labels=["x","y","z"], title="amplitude function
  |2,1,3/2,3/2>, component 3, real part",
     titlefont=[TIMES,BOLD,14], view=[-14..14,-14..14,-14..14]);
```

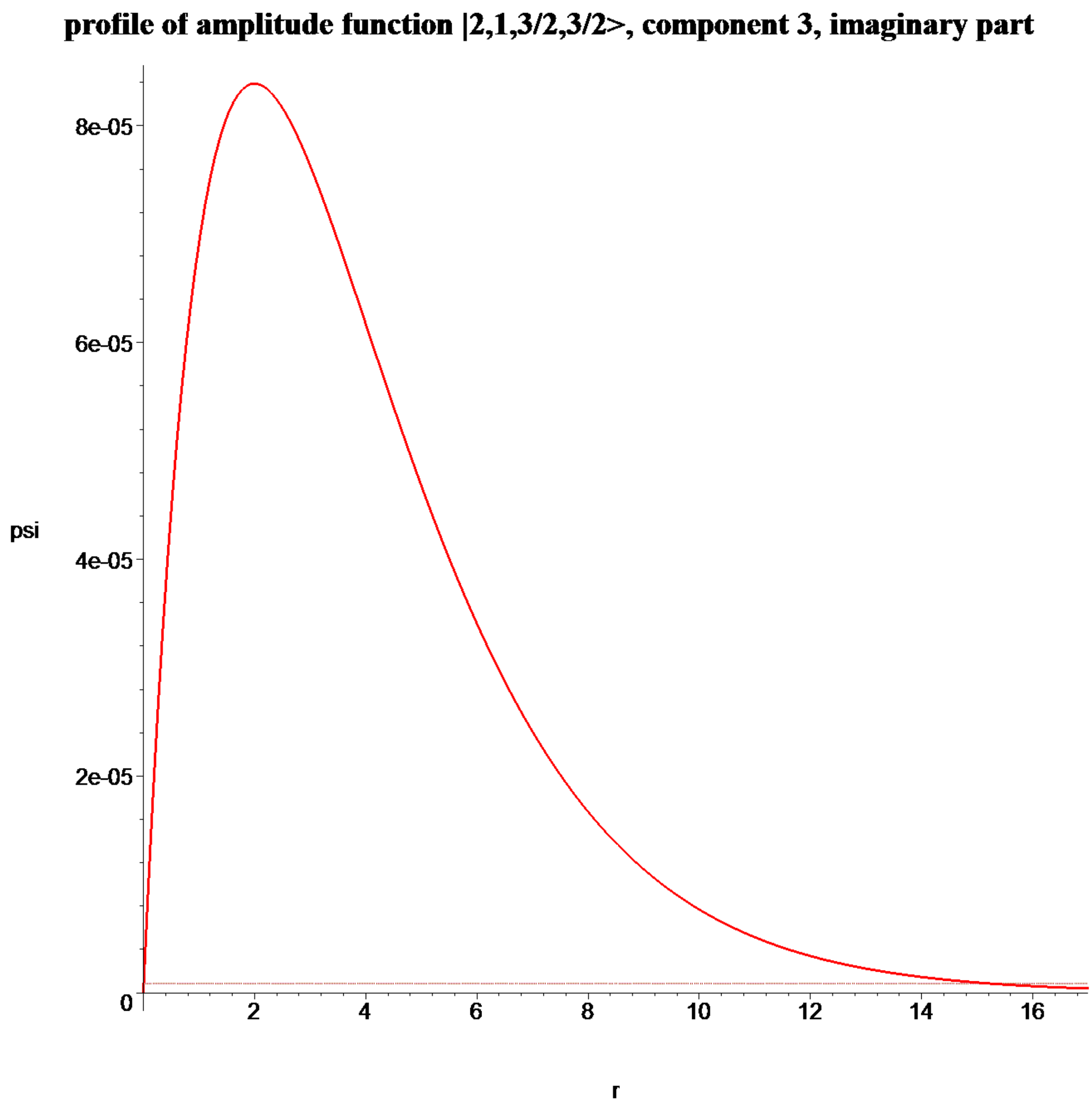
amplitude function |2,1,3/2,3/2>, component 3, real part




```
>
```

we plot next the radial profile of the imaginary part along the polar axis, for which $\theta = 0$, to obtain the criterion for the surface,

```
> plot([eval(ip, [theta=Pi/4,phi=0,op(cond)]), 8.4e-7],
      r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,3/2,3/2>,
  component 3, imaginary part",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

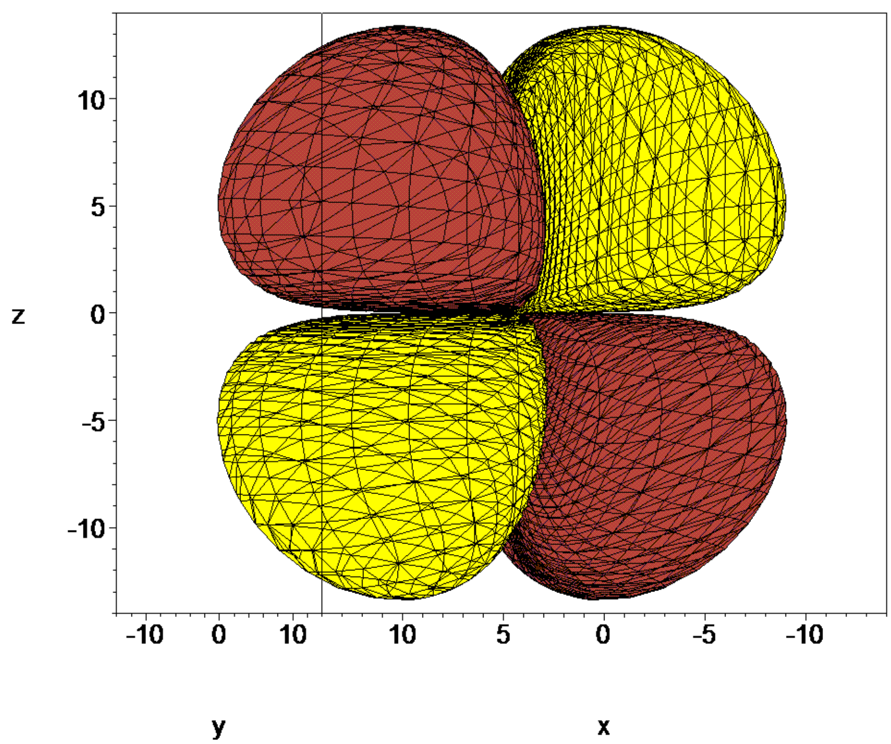


>

and then the surface itself.

```
> plots[implicitplot3d]([eval(ip, cond)=8.4e-7, eval(ip,
  cond)=-8.4e-7], r=0..17,
     theta=0..Pi, phi=0..2*Pi, colour=[brown, yellow],
  orientation=[70,90],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |2,1,3/2,3/2>, component 3,
  imaginary part",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
  view=[-14..14,-14..14,-14..14]);
```

amplitude function |2,1,3/2,3/2>, component 3, imaginary part




```
>
```

These two surfaces resemble those of the corresponding real and imaginary parts of $\psi_{0,2,1}(r, \theta, \phi)$. The fourth component has both real and imaginary parts,

```
> '`|2,1,3/2,3/2>`'[4] = evalc(`|2,1,3/2,3/2>`[4]);
```

$$|2,1,3/2,3/2>_4 = -\frac{1}{32}\alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2 \sin(2\phi) + \frac{1}{32} I \alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2 \cos(2\phi)$$

```
> rp := Re(`|2,1,3/2,3/2>`[4]) assuming real;
```

$$rp := -\frac{1}{32}\alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2 \sin(2\phi)$$

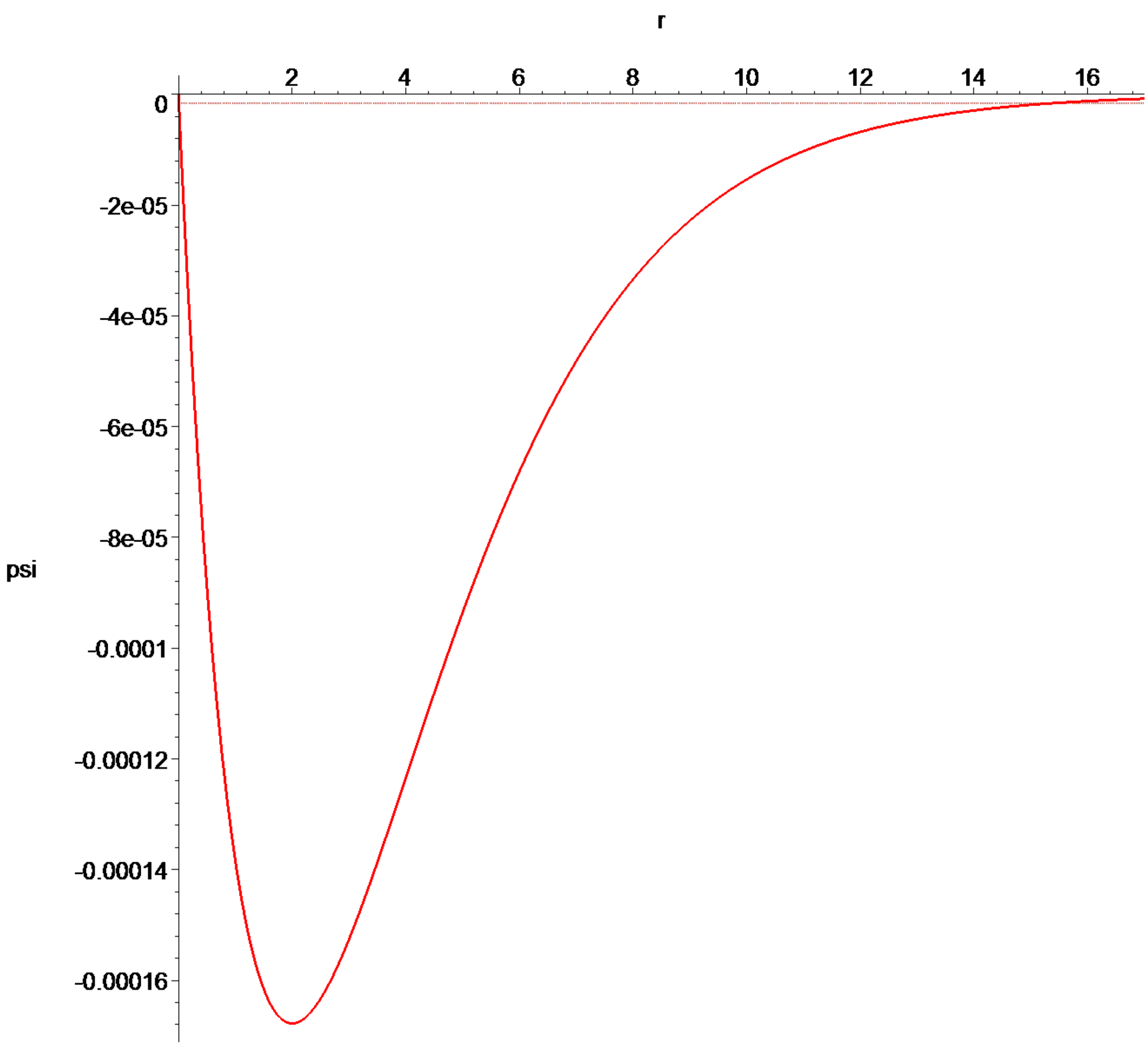
```
> ip := Im(`|2,1,3/2,3/2>`[4]) assuming real;
```

$$ip := \frac{1}{32}\,\alpha\, Z\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2 \cos(2\,\phi)$$

we plot next the radial profile of the real component along the polar axis, for which $\theta = \frac{\pi}{2}$, to obtain the criterion for the surface,

```
> plot([eval(rp, [theta=Pi/2,phi=Pi/4,op(cond)]), -1.6e-6],
     r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
     title="profile of amplitude function |2,1,3/2,3/2>,
  component 4, real part",
     linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

profile of amplitude function |2,1,3/2,3/2>, component 4, real part

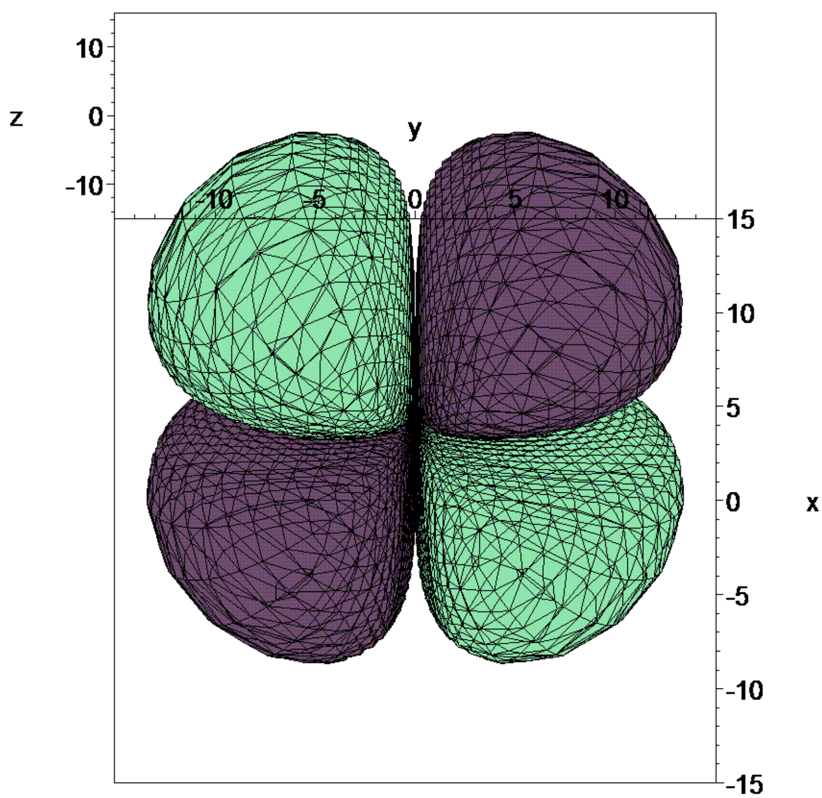


>

We plot the surface itself in its real part.

```
> plots[implicitplot3d]([eval(rp, cond)=1.67e-6, eval(rp, cond)=-1.67e-6], r=0..17, theta=0..Pi,
    phi=0..2*Pi, colour=[aquamarine, violet], orientation=[0,160], labels=["x","y","z"],
    coords = scispherical, grid=[30,30,30], scaling=constrained, axes=box,
    title="amplitude function |2,1,3/2,3/2>, component 4, real part",
    titlefont=[TIMES,BOLD,14], view=[-15..15,-15..15,-15..15]);
```

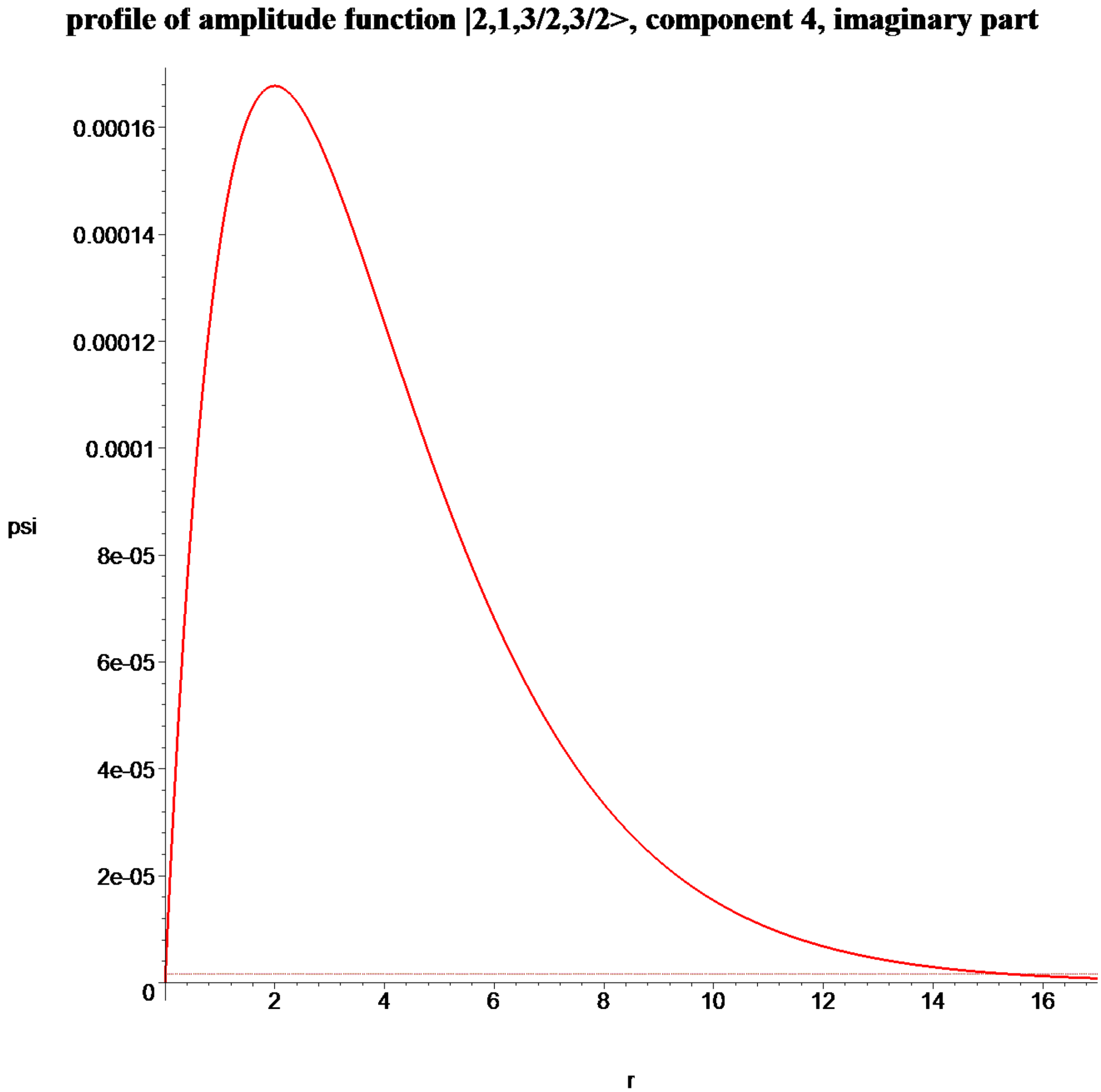
amplitude function |2,1,3/2,3/2>, component 4, real part



>

For the profile of the imaginray component, to obtain the criterion for the surface,

```
> plot([eval(ip, [theta=Pi/2,phi=0,op(cond)]), 1.67e-6],
    r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
     title="profile of amplitude function |2,1,3/2,3/2>,
  component 4, imaginary part",
     linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```



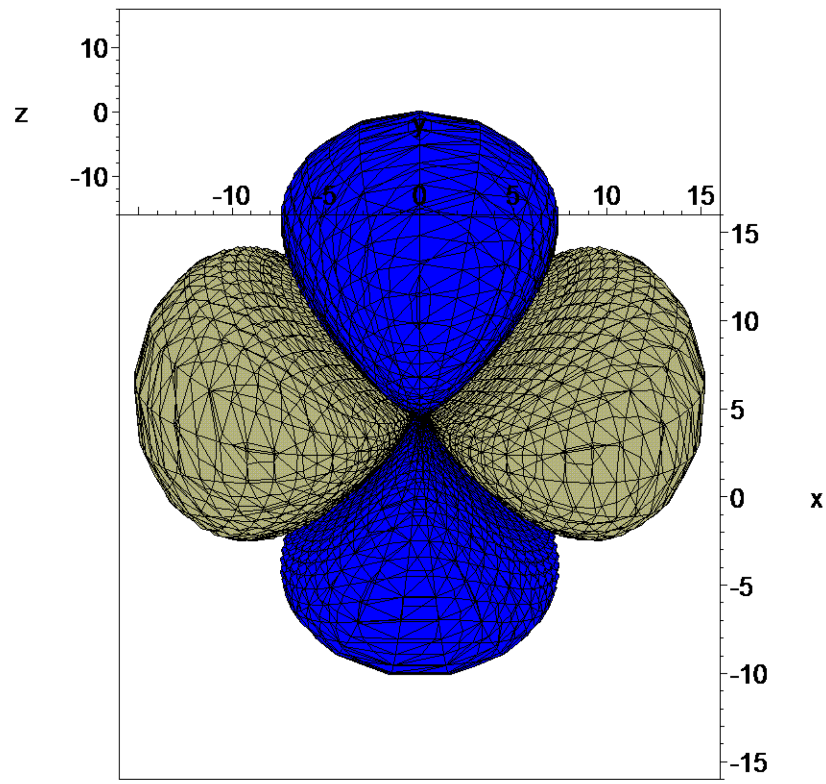

```
>
```

We plot the surface itself in its imaginary part.

```
> plots[implicitplot3d]([eval(ip, cond)=1.67e-6, eval(ip,
  cond)=-1.67e-6], r=0..17,
    theta=0..Pi, phi=0..2*Pi, colour=[blue, khaki],
  orientation=[0,160],
    coords = scispherical, grid=[30,30,30], scaling=constrained,
```

```
axes=box,
   title="amplitude function |2,1,3/2,3/2>, component 4,
imaginary part",
   labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
view=[-16..16,-16..16,-16..16]);
```

amplitude function |2,1,3/2,3/2>, component 4, imaginary part




```
>
```

The latter two plots resemble the corresponding real and imaginary parts of $\psi_{0,\,2,\,-2}(r,\,\theta,\,\phi)$. From |2,1,3/2,3/2>,

```
> p := evalc(`|2,1,3/2,3/2>`);
```

$$p := \left[\begin{array}{c} \frac{1}{8} r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\phi) + \frac{1}{8} I r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\sin(\phi) \\ 0 \\ -\frac{1}{32}\alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\sin(\phi) + \frac{1}{32} I \alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\cos(\phi) \\ -\frac{1}{32}\alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2 \sin(2\phi) + \frac{1}{32} I \alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2 \cos(2\phi) \end{array}\right]$$

and its complex conjugate,

```
> pc := evalc(subs(I=-I,`|2,1,3/2,3/2>`));
```

$$pc := \left[\begin{array}{c} \frac{1}{8} r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\phi) - \frac{1}{8} I r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\sin(\phi) \\ 0 \\ -\frac{1}{32}\alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\sin(\phi) - \frac{1}{32} I \alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\cos(\phi) \\ -\frac{1}{32}\alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2 \sin(2\phi) - \frac{1}{32} I \alpha Z r \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)^2 \cos(2\phi) \end{array}\right]$$

we form product |2,1,1/2,1/2>* **.** |2,1,1/2,1/2>,

```
> ps :=
  evalc(simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,3/2,3/2
  >`)) . `|2,1,3/2,3/2>`)) assuming real;
```

$$ps := \frac{1}{1024}\sin(\theta)^2 (Z^2\alpha^2 + 16) r^2 \mathbf{e}^{(-r)}$$

which we separate into the two parts.

```
> fl := simplify(remove(has, expand(ps), alpha));
```

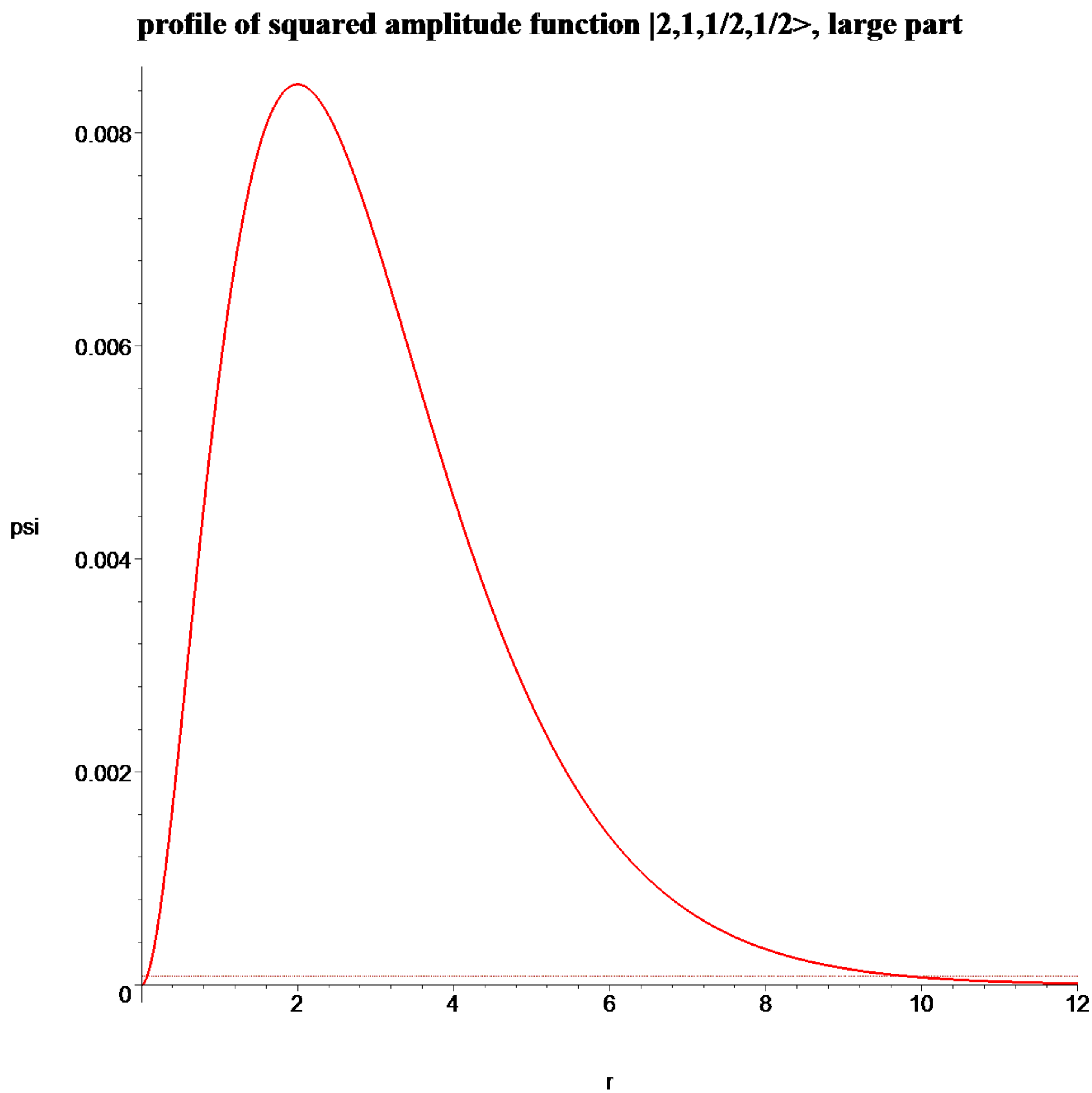
$$fl := \frac{1}{64}\sin(\theta)^2 r^2 \mathbf{e}^{(-r)}$$

```
> fs := simplify(ps - fl);
```

$$fs := \frac{1}{1024}\sin(\theta)^2 r^2 \mathbf{e}^{(-r)} Z^2 \alpha^2$$

We plot the radial profile of the large part of squared |2,1,3/2,3/2>,

```
> plot([eval(fl, [op(cond), theta=Pi/2]), 8.6e-5], r=0..12,
        title="profile of squared amplitude function
  |2,1,1/2,1/2>, large part",
        titlefont=[TIMES,BOLD,14], colour=[red, brown, green],
  linestyle=[1,2],
        labels=["r", "psi"], thickness=[3,2]);
```

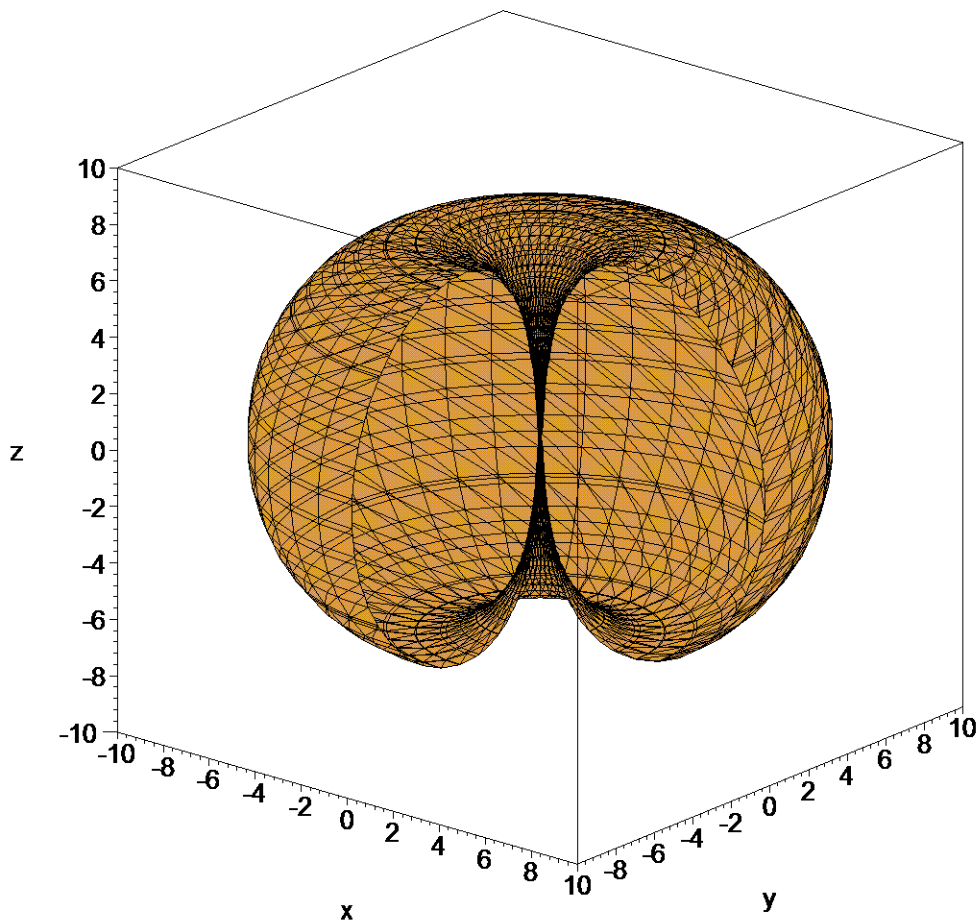



```
>
```

and its surface,

```
> plots[implicitplot3d](eval(f1, cond)=8.6e-5, r=0..13,
  theta=0..Pi, phi=0..3/2*Pi,
     colour=gold, orientation=[-50,70], labels=["x","y","z"],
  coords = scispherical,
     scaling=constrained, title="squared amplitude function
  |2,1,3/2,3/2>, large part",
     grid=[30,30,30], axes=box, titlefont=[TIMES,BOLD,14],
  view=[-10..10,-10..10,-10..10]);
```

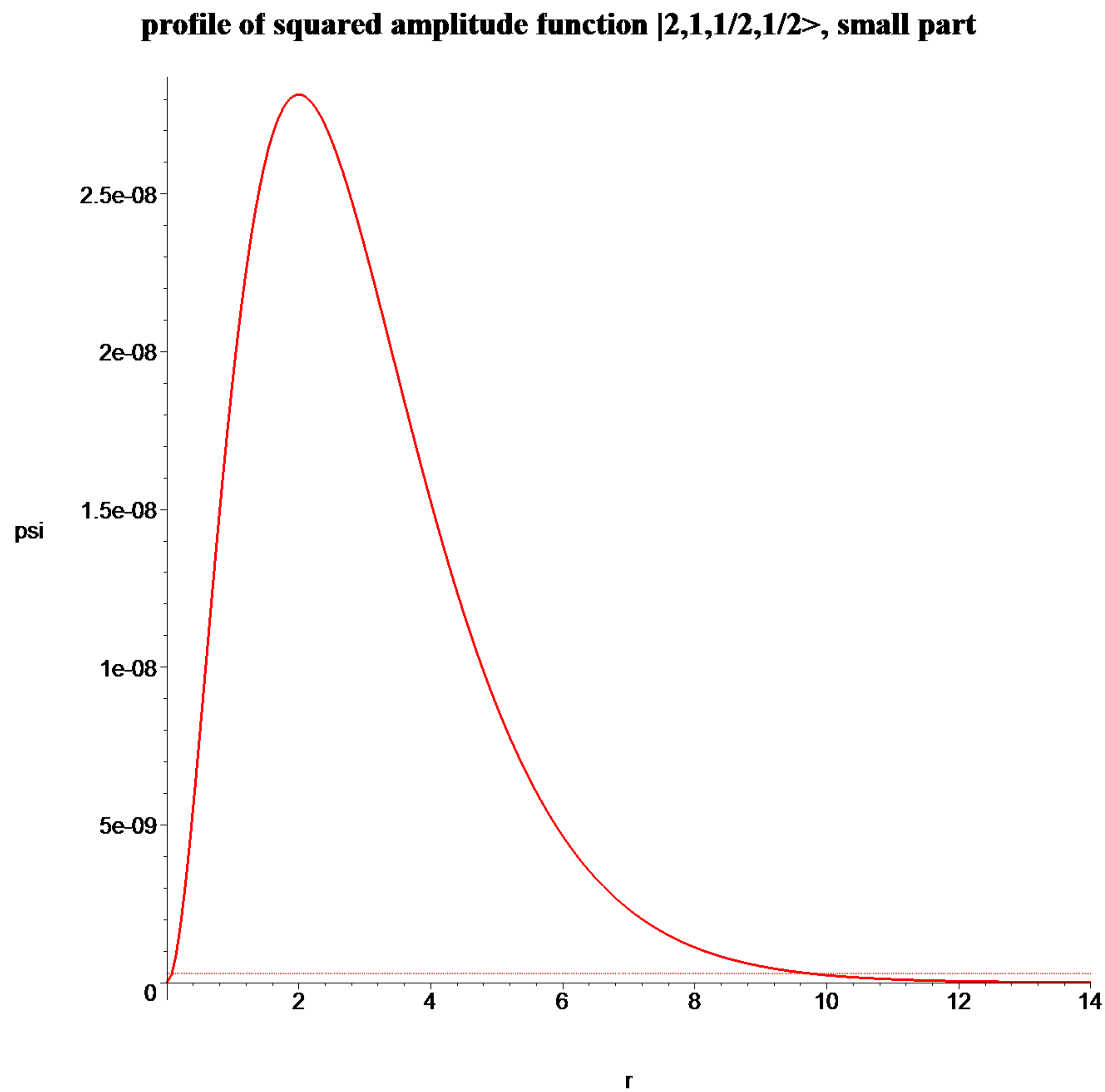
squared amplitude function |2,1,3/2,3/2>, large part




```
>
```

which exhibits one toroidal lobe.   We plot the radial profile along the polar axis of the small part.

```
> plot([eval(fs, [op(cond), theta=Pi/2]), 2.8e-10], r=0..14,
     title="profile of squared amplitude function |2,1,1/2,1/2>,
  small part",
     titlefont=[TIMES,BOLD,14], colour=[red, brown],
  linestyle=[1,2],
     labels=["r", "psi"], thickness=[3,2]);
```

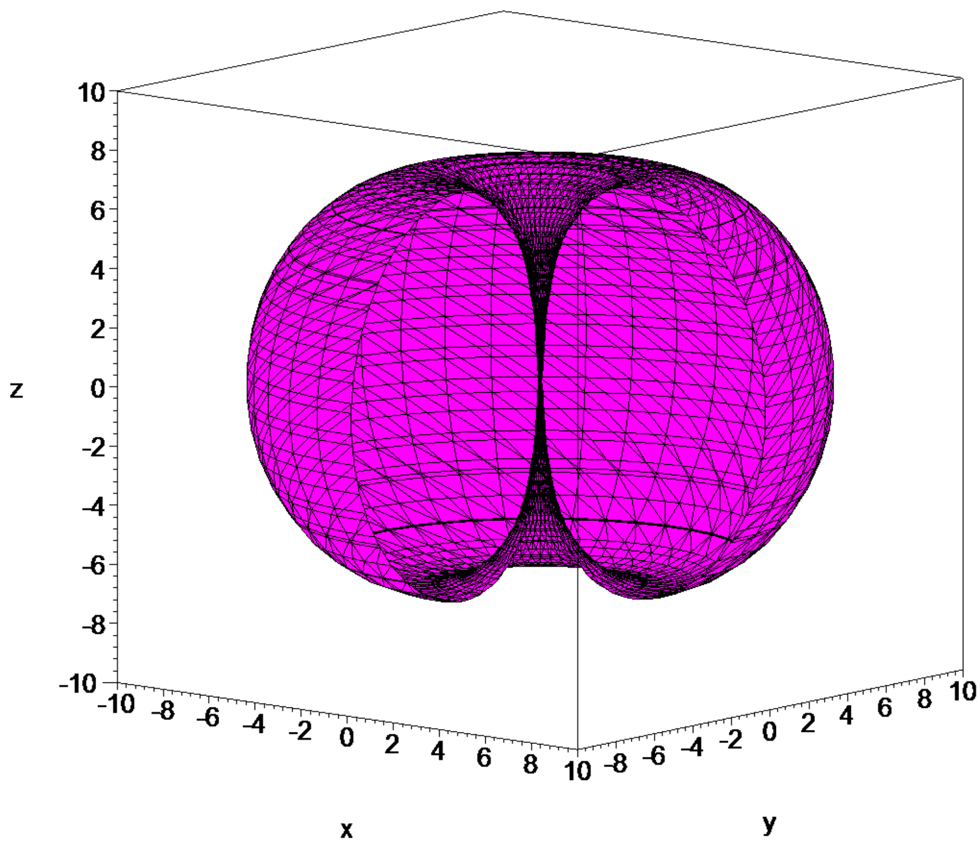



```
>
```

We accordingly plot the surface of the small part of |2,1,3/2,3/2> squared.

```
> plots[implicitplot3d](eval(fs, cond)=2.8e-10, r=0..12,
  theta=0..Pi, phi=0..3/2*Pi,
     colour=magenta, orientation=[-50,80],coords = scispherical,
  grid=[30,30,30], axes=box,
     scaling=constrained, title="squared amplitude function
  |2,1,3/2,3/2>, small part",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
  view=[-10..10,-10..10,-10..10]);
```

squared amplitude function |2,1,3/2,3/2>, small part




```
>
```

The two tori of the large and small parts have the same geometric shape and size according to the criterion for their plots and resemble $\psi_{0,\,1,\,1}(r,\,\theta,\,\phi)^2$ or $\psi_{0,\,1,\,-1}(r,\,\theta,\,\phi)^2$, which are identical.

We proceed to investigate |2,1,3/2,1/2>,

```
> '`|2,1,3/2,1/2>`' = `|2,1,3/2,1/2>`;
```

$$|2,1,3/2,1/2> = \begin{bmatrix} \frac{1}{24}\sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \cos(\theta) \\ -\frac{1}{48}\sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\, \mathbf{e}^{(\phi I)} \\ \frac{1}{64} I \sqrt{2}\sqrt{6}\, \alpha Z r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \left(\cos(\theta)^2 - \frac{1}{2}\right) \\ \frac{1}{64} I \sqrt{2}\sqrt{6}\, \alpha Z r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\theta)\, \mathbf{e}^{(\phi I)} \end{bmatrix}$$

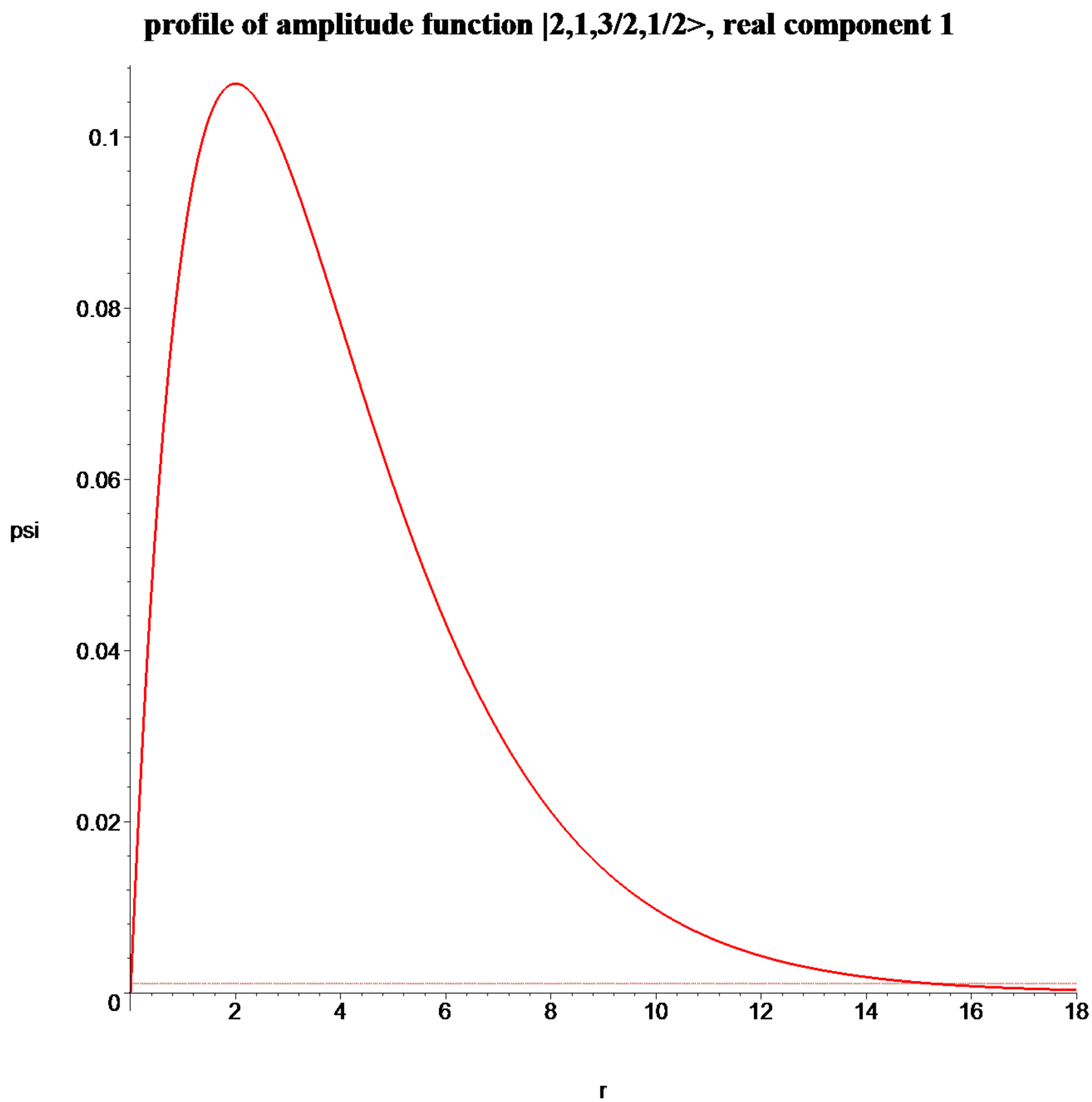
which has four non-zero components. For the first component of |2,1,3/2,1/2> ,

```
> '`|2,1,3/2,1/2>`'[1] = `|2,1,3/2,1/2>`[1];
```

$$|2,1,3/2,1/2>_1 = \frac{1}{24}\sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \cos(\theta)$$

which is real, we plot the radial profile.

```
> plot([eval(`|2,1,3/2,1/2>`[1], theta=0), 0.00107], r=0..18,
    title="profile of amplitude function |2,1,3/2,1/2>, real
  component 1",
    titlefont=[TIMES,BOLD,14], colour=[red, brown],
  linestyle=[1,2],
    labels=["r", "psi"], thickness=[3,2]);
```



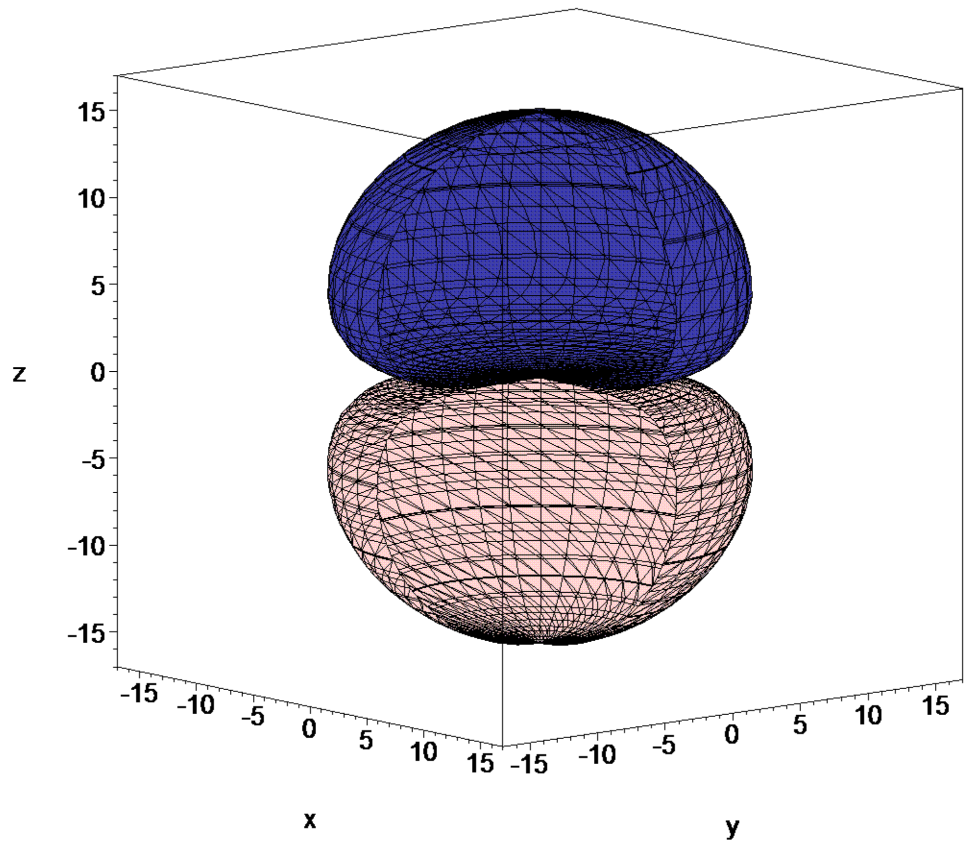
>

We plot the surface of this real first component of |2,1,3/2,1/2> at a value of ψ that is $\frac{1}{100}$ of its maximum magnitude, cut open to show the lack of an inner lobe,

```
> plots[implicitplot3d]([`|2,1,3/2,1/2>`[1]=0.00107,
  `|2,1,3/2,1/2>`[1]=-0.00107],
     r=0..18, theta=0..Pi, phi=0..3/2*Pi, colour=[navy, pink],
  labels=["x","y","z"],
     orientation=[-40,80], coords = scispherical,
  grid=[30,30,30], scaling=constrained,
     axes=box, title="amplitude function |2,1,3/2,1/2>, real
  component 1",
```

```
titlefont=[TIMES,BOLD,14], view=[-17..17,-17..17,-17..17]);
```

amplitude function |2,1,3/2,1/2>, real component 1




```
>
```

The second component of |2,1,3/2,1/2> has real and imaginary parts;

```
> '`|2,1,3/2,1/2>`'[2] = evalc(`|2,1,3/2,1/2>`[2]);
```

$$|2,1,3/2,1/2>_2 = -\frac{1}{48}\sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\phi) - \frac{1}{48} I \sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\sin(\phi)$$

```
> rp := Re(`|2,1,3/2,1/2>`[2]) assuming real;
```

$$rp := -\frac{1}{48}\sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \sin(\theta)\cos(\phi)$$

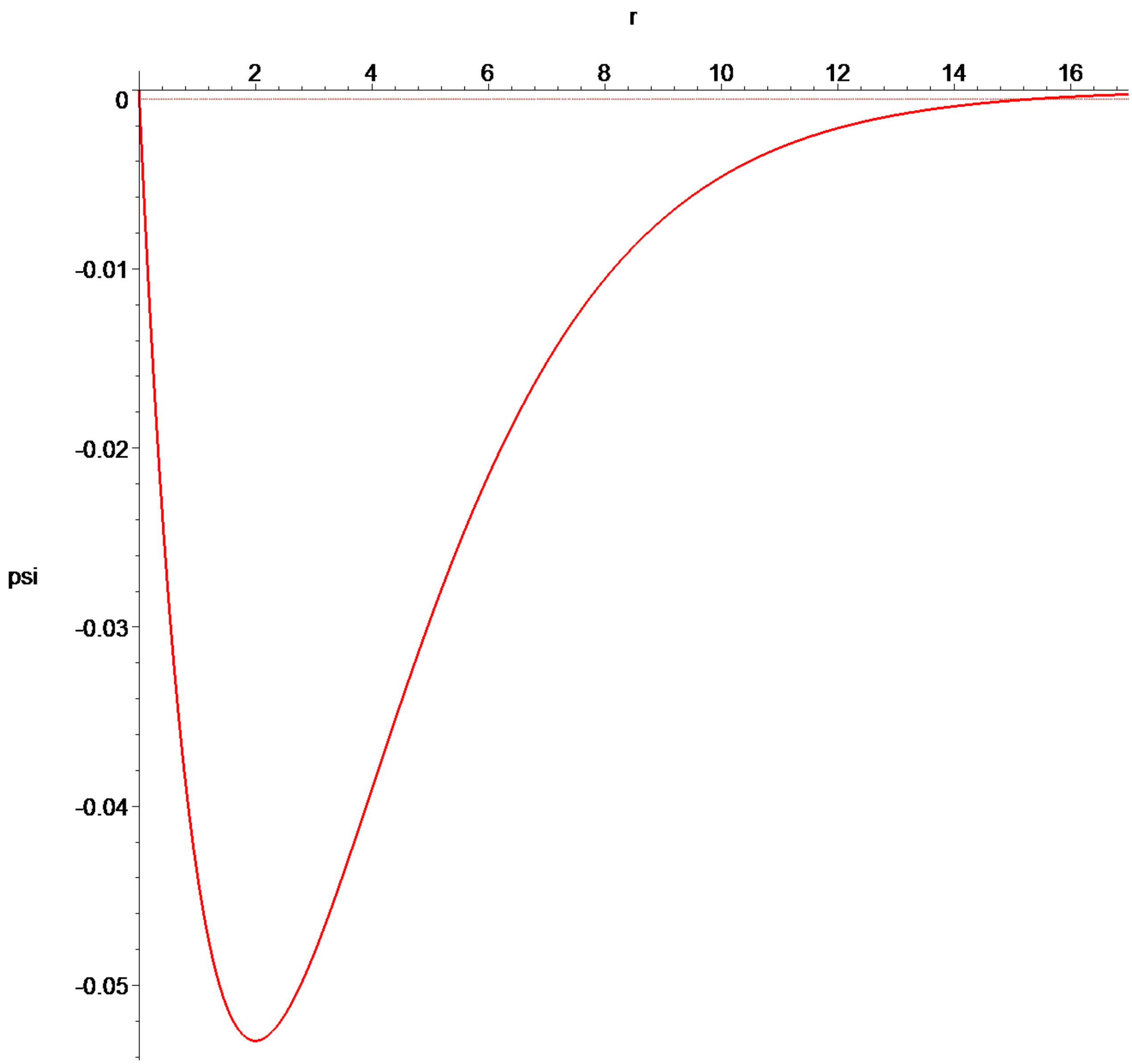
```
> ip := Im(`|2,1,3/2,1/2>`[2]) assuming real;
```

$$ip := -\frac{1}{48}\sqrt{2}\,\sqrt{6}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\sin(\phi)$$

we plot first the radial profile of the real part along the polar axis, for which θ = 0, to obtain the criterion for the surface,

```
> plot([eval(rp, [theta=Pi/2,phi=0]), -0.00053],
     r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
     title="profile of amplitude function |2,1,1/2,1/2>,
  component 2, real part",
     linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

profile of amplitude function |2,1,1/2,1/2>, component 2, real part

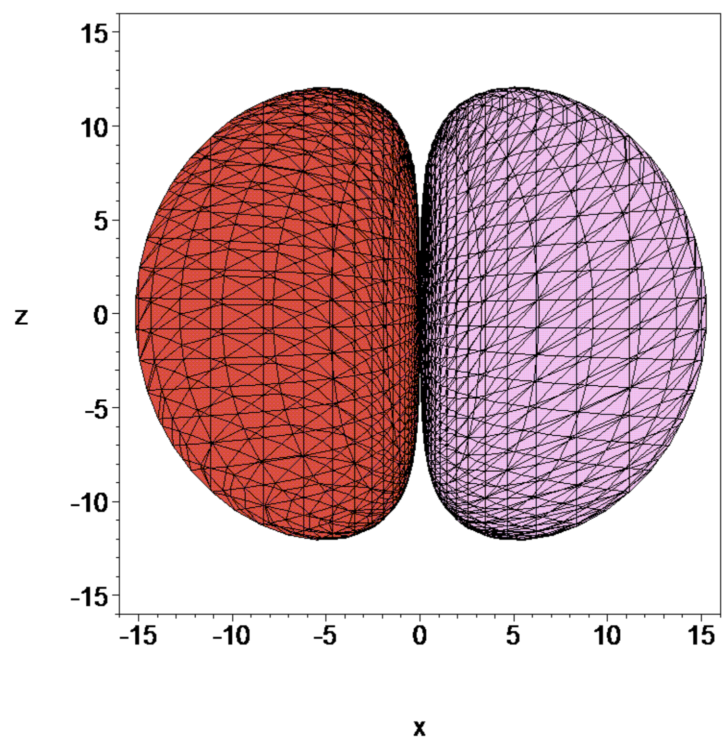


>

and then the surface itself.

```
> plots[implicitplot3d]([rp=5.3e-4, rp=-5.3e-4], r=0..17,
  theta=0..Pi, phi=0..2*Pi,
     colour=[orange, plum], orientation=[-90,90],
  labels=["x","y","z"],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |2,1,3/2,1/2>, component 2, real
  part",
     titlefont=[TIMES,BOLD,14], view=[-16..16,-16..16,-16..16]);
```

amplitude function |2,1,3/2,1/2>, component 2, real part

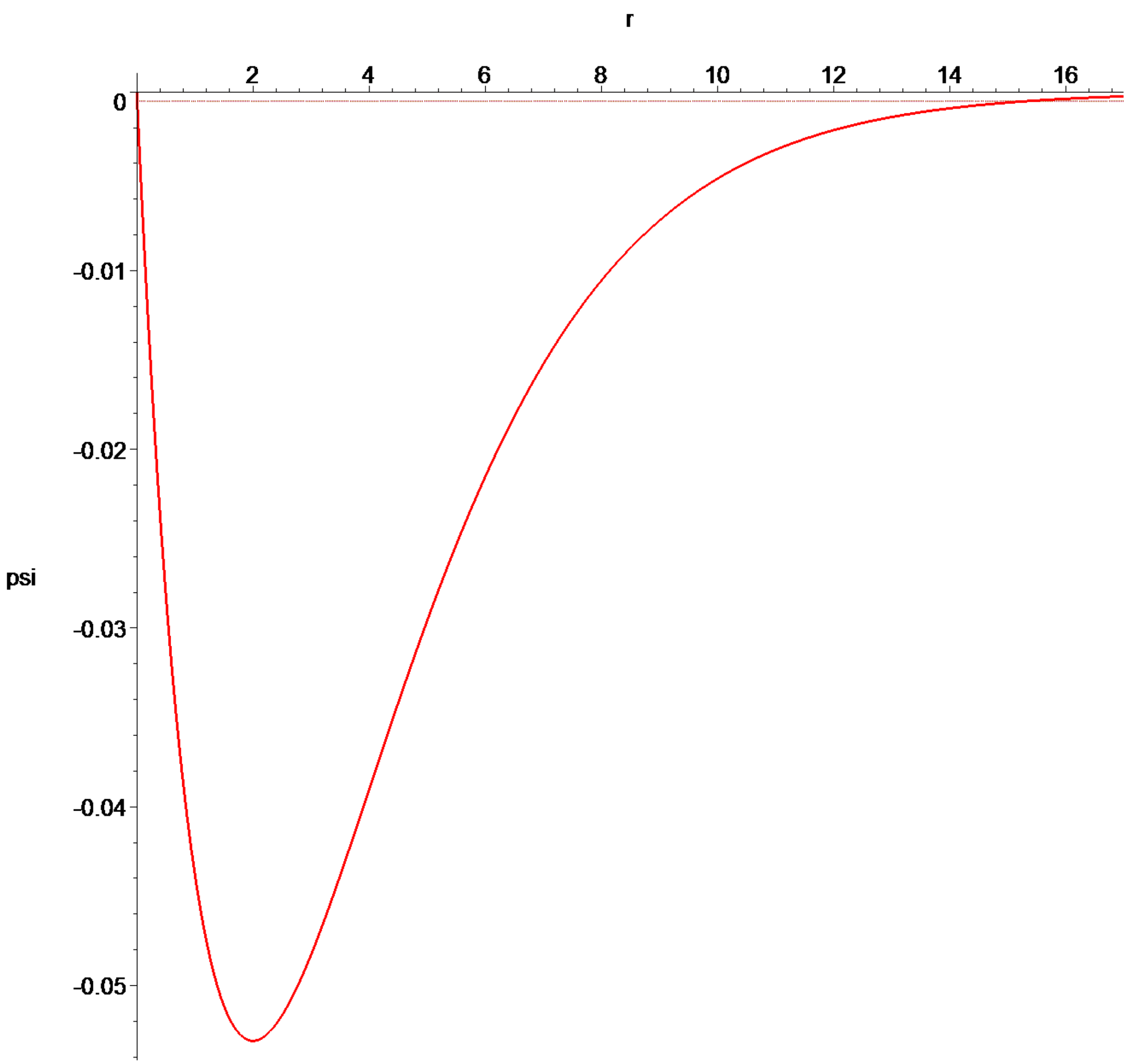


>

we plot next the profile of the imaginary part along the polar axis, for which $\theta = 0$, to obtain the criterion for the surface,

```
> plot([eval(ip, [theta=Pi/2,phi=Pi/2]), -5.3e-4],
      r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,3/2,1/2>,
  component 2, imaginary part",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

profile of amplitude function |2,1,3/2,1/2>, component 2, imaginary part



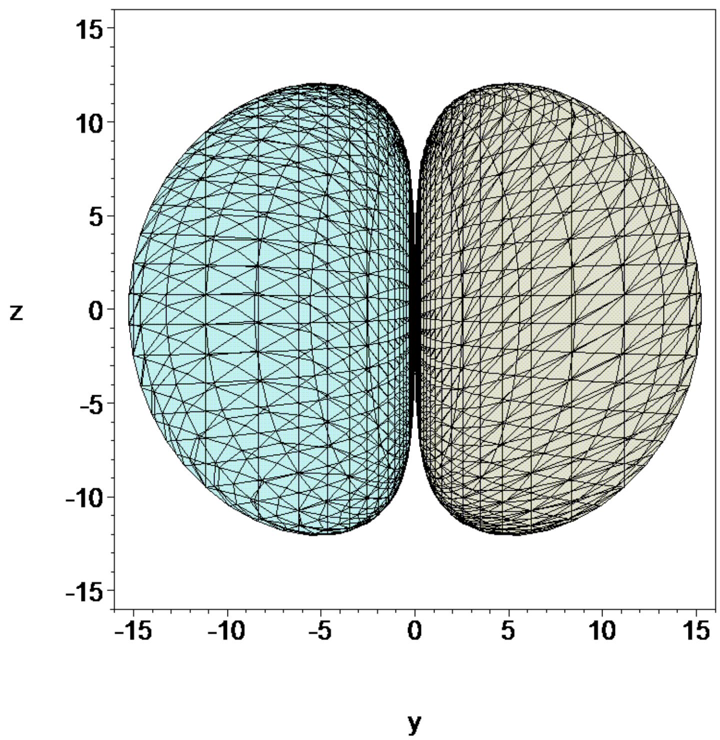

```
>
```

and then the surface itself.

```
> plots[implicitplot3d]([ip=5.3e-4, ip=-5.3e-4], r=0..17,
     theta=0..Pi, phi=0..2*Pi, colour=[turquoise, wheat],
  orientation=[0,90],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
```

```
   title="amplitude function |2,1,3/2,1/2>, component 2,
imaginary part",
   labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
view=[-16..16,-16..16,-16..16]);
```

amplitude function |2,1,3/2,1/2>, component 2, imaginary part



>

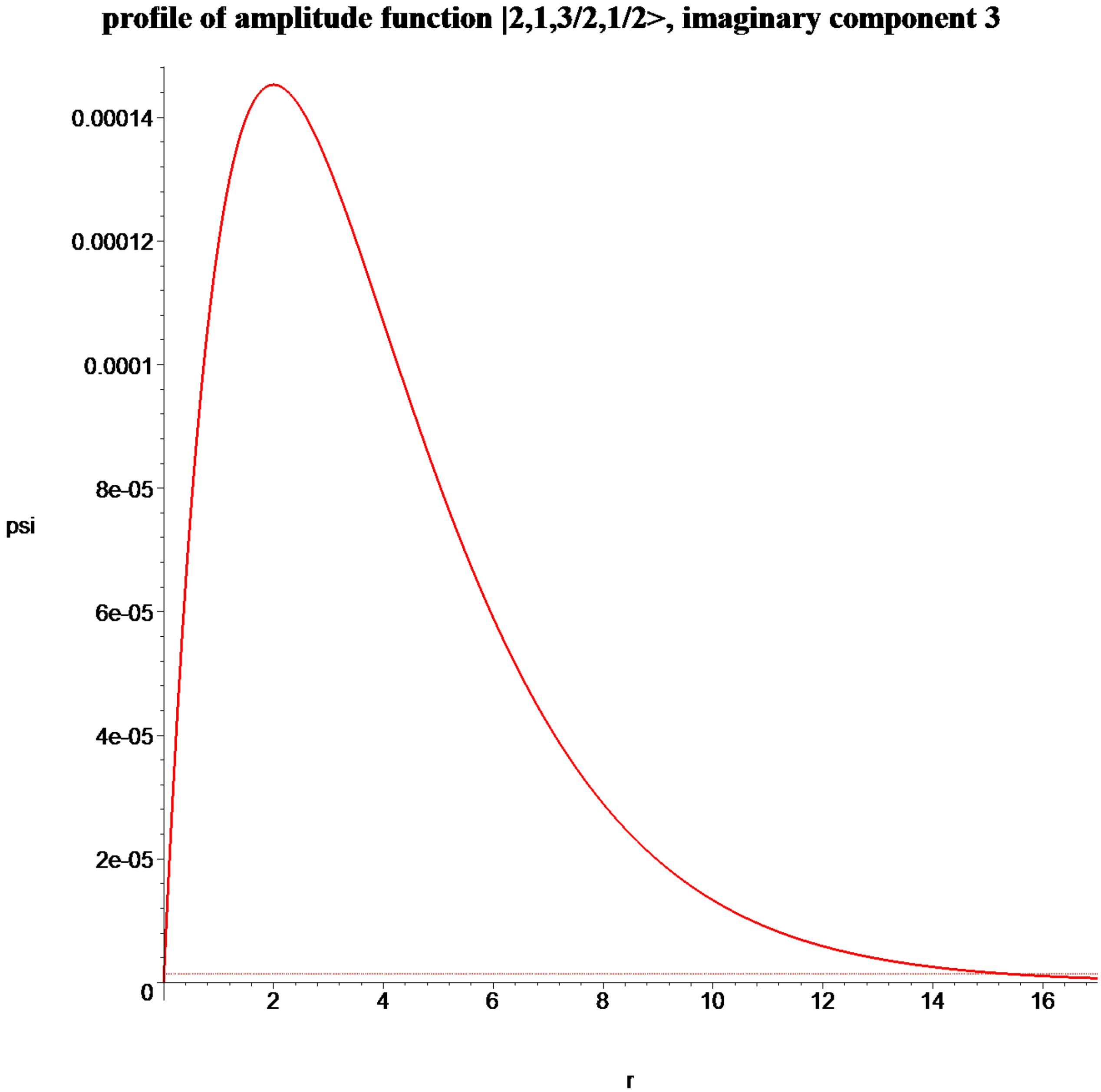
The latter two surfaces resemble the corresponding surfaces of the real and imaginary parts of $\psi_{0,\,1,\,-1}(r, \theta, \phi)$. The third component has only an imaginary part;

```
> '`|2,1,3/2,1/2>`'[3] = evalc(`|2,1,3/2,1/2>`[3]);
```

$$|2,1,3/2,1/2>_3 = \frac{1}{64} I \sqrt{2}\,\sqrt{6}\,\alpha\, Z\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)} \left(\cos(\theta)^2 - \frac{1}{2}\right)$$

we plot next the profile along the polar axis, for which $\theta = \frac{\pi}{2}$, to obtain the criterion for the surface,

```
> plot([eval(Im(`|2,1,3/2,1/2>`[3]), [theta=0,op(cond)]),
  1.45e-6],
      r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,3/2,1/2>,
  imaginary component 3",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```



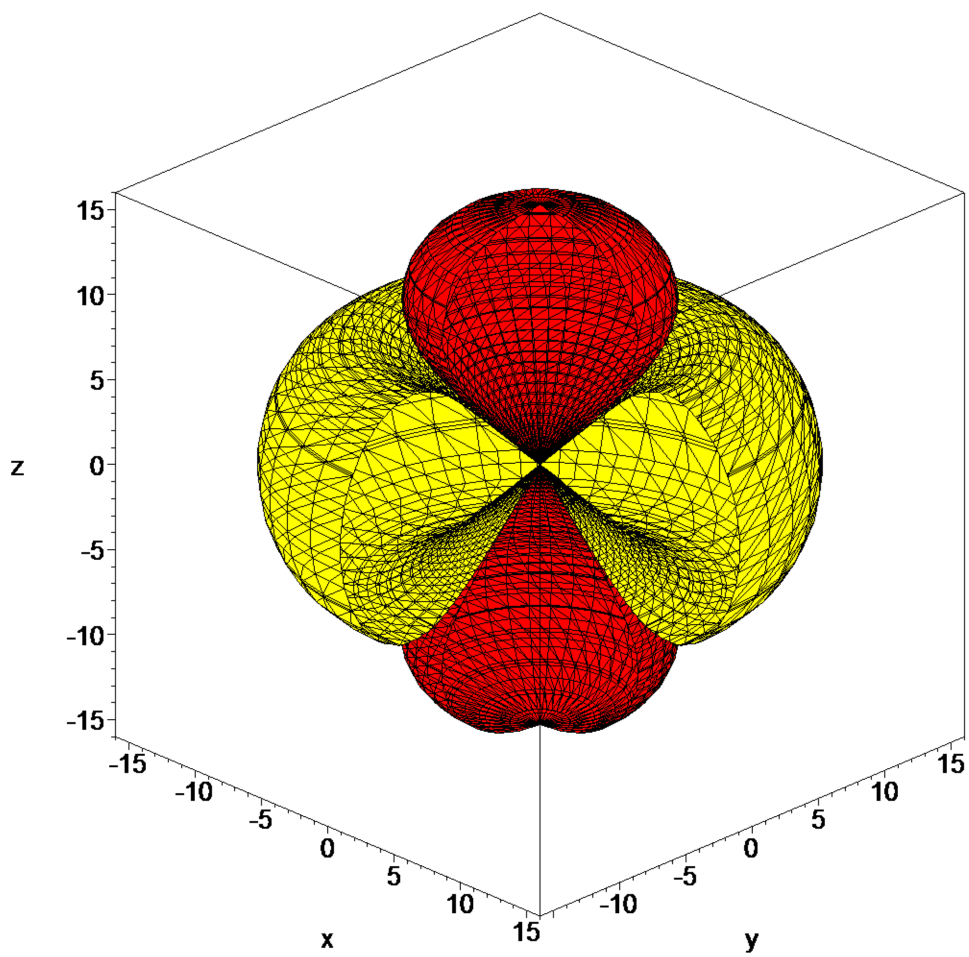

```
>
```

We plot the surface of this imaginary part, cut open to reveal the inner structure.

```
> plots[implicitplot3d]([eval(Im(`|2,1,3/2,1/2>`[3]),
```

```
cond)=1.45e-6,
   eval(Im(`|2,1,3/2,1/2>`[3]), cond)=-1.6e-6], r=0..17,
theta=0..Pi,
   phi=0..3/2*Pi, colour=[red, yellow], orientation=[-45,65],
labels=["x","y","z"],
   coords = scispherical, grid=[30,30,30], scaling=constrained,
axes=box,
   title="amplitude function |2,1,3/2,1/2>, imaginary component
3",
   titlefont=[TIMES,BOLD,14], view=[-16..16,-16..16,-16..16]);
```

amplitude function |2,1,3/2,1/2>, imaginary component 3



>

This surface resembles that of the real surface of $\psi_{0,\,2,\,0}(r, \theta, \phi)$. The fourth component of

|2,1,3/2,1/2> has real and imaginary parts;

```
> '`|2,1,3/2,1/2>`'[4] = evalc(`|2,1,3/2,1/2>`[4]);
```

$$|2,1,3/2,1/2>_4 = -\frac{1}{64}\sqrt{2}\,\sqrt{6}\,\alpha\,Z\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\sin(\phi) + \frac{1}{64}I\sqrt{2}\,\sqrt{6}\,\alpha\,Z\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\cos(\phi)$$

```
> rp := Re(`|2,1,3/2,1/2>`[4]) assuming real;
```

$$rp := -\frac{1}{64}\sqrt{2}\,\sqrt{6}\,\alpha\,Z\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\sin(\phi)$$

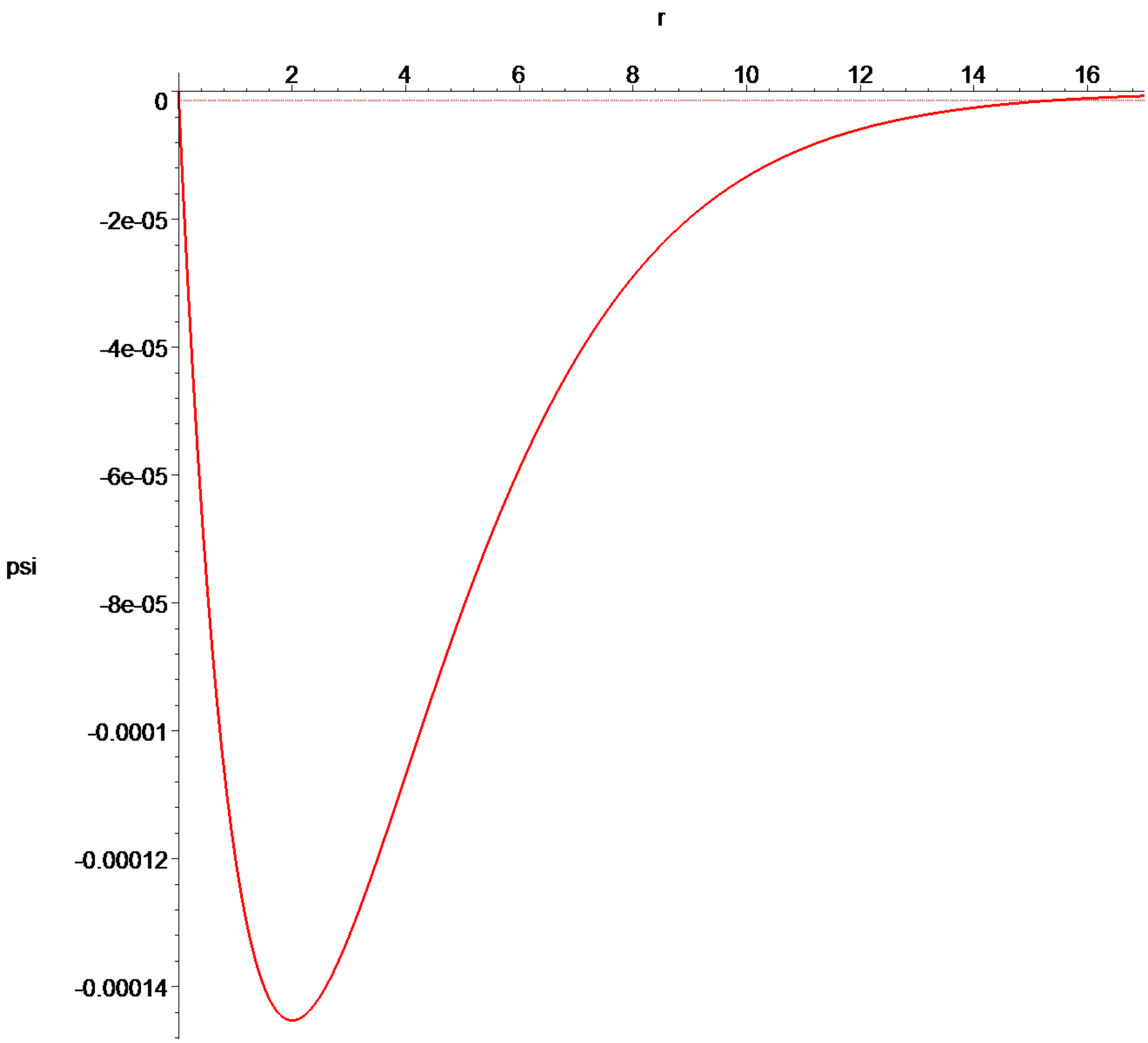
```
> ip := Im(`|2,1,3/2,1/2>`[4]) assuming real;
```

$$ip := \frac{1}{64}\sqrt{2}\,\sqrt{6}\,\alpha\,Z\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\cos(\phi)$$

we plot first the profile of the real part along the polar axis, for which $\theta = 0$, to obtain the criterion for the surface,

```
> plot([eval(rp, [theta=Pi/4,phi=Pi/2,op(cond)]), -1.45e-6],
      r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,3/2,1/2>,
  component 4, real part",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

profile of amplitude function |2,1,3/2,1/2>, component 4, real part

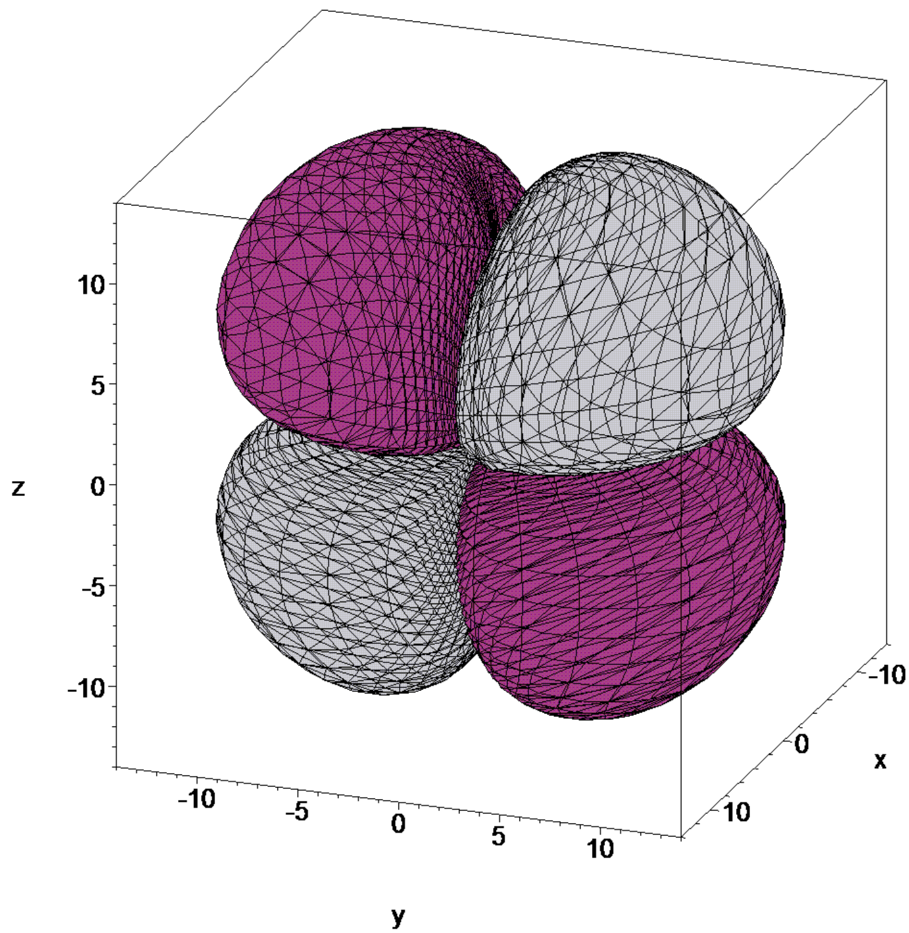


>

and then the surface itself.

```
> plots[implicitplot3d]([eval(rp, cond)=1.45e-6,  eval(rp,
  cond)=-1.45e-6],
     r=0..17, theta=0..Pi, phi=0..2*Pi, colour=[maroon, grey],
  orientation=[20,70],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     labels=["x","y","z"], title="amplitude function
  |2,1,3/2,1/2>, component 4, real part",
     titlefont=[TIMES,BOLD,14], view=[-14..14,-14..14,-14..14]);
```

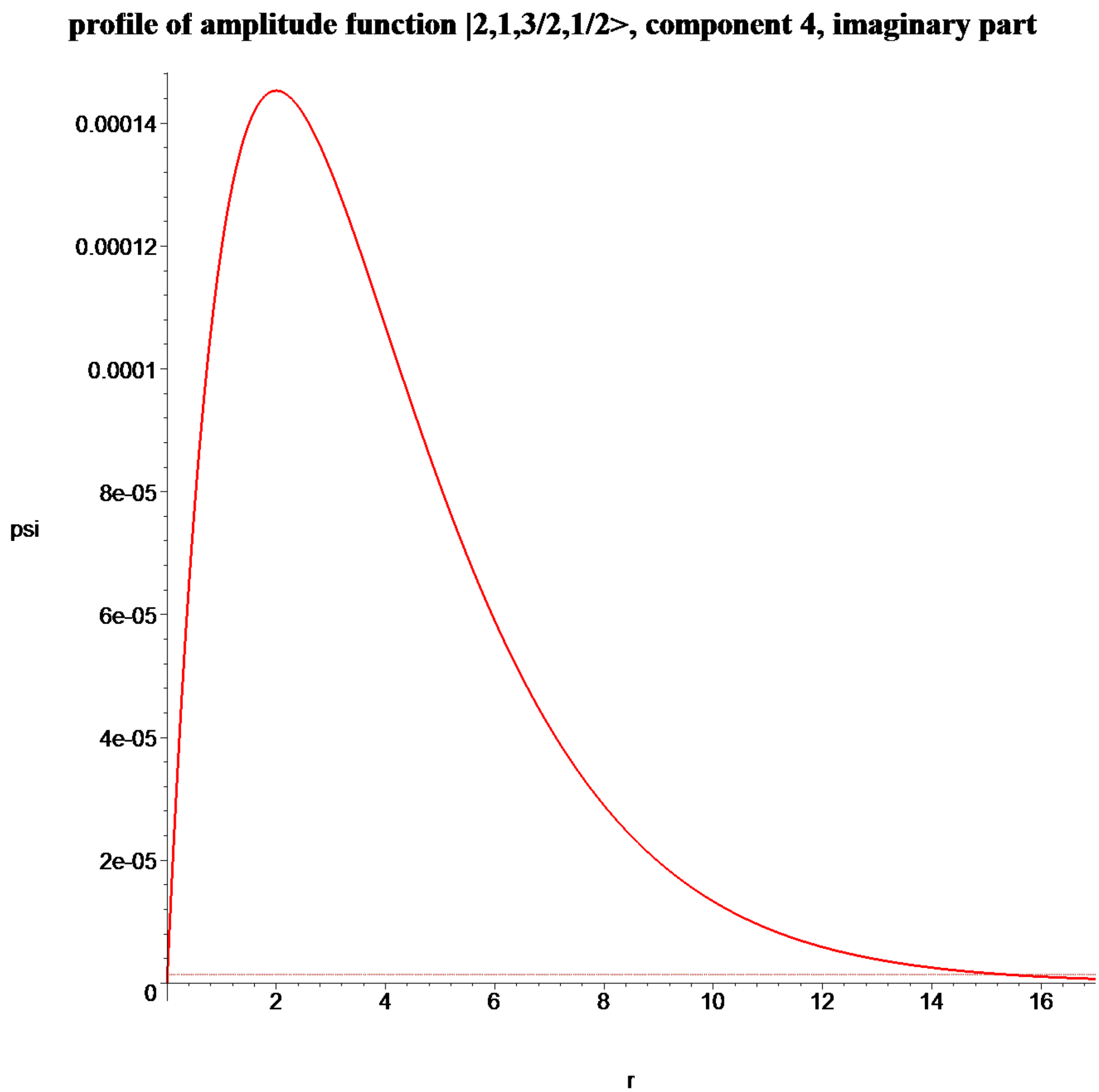
amplitude function |2,1,3/2,1/2>, component 4, real part




```
>
```

we plot next the profile of the imaginary part along the polar axis, for which θ = 0, to obtain the criterion for the surface,

```
> plot([eval(ip, [theta=Pi/4,phi=0,op(cond)]), 1.45e-6],
      r=0..17, titlefont=[TIMES,BOLD,14], colour=[red, brown],
      title="profile of amplitude function |2,1,3/2,1/2>,
  component 4, imaginary part",
      linestyle=[1,2], labels=["r", "psi"], thickness=[3,2]);
```

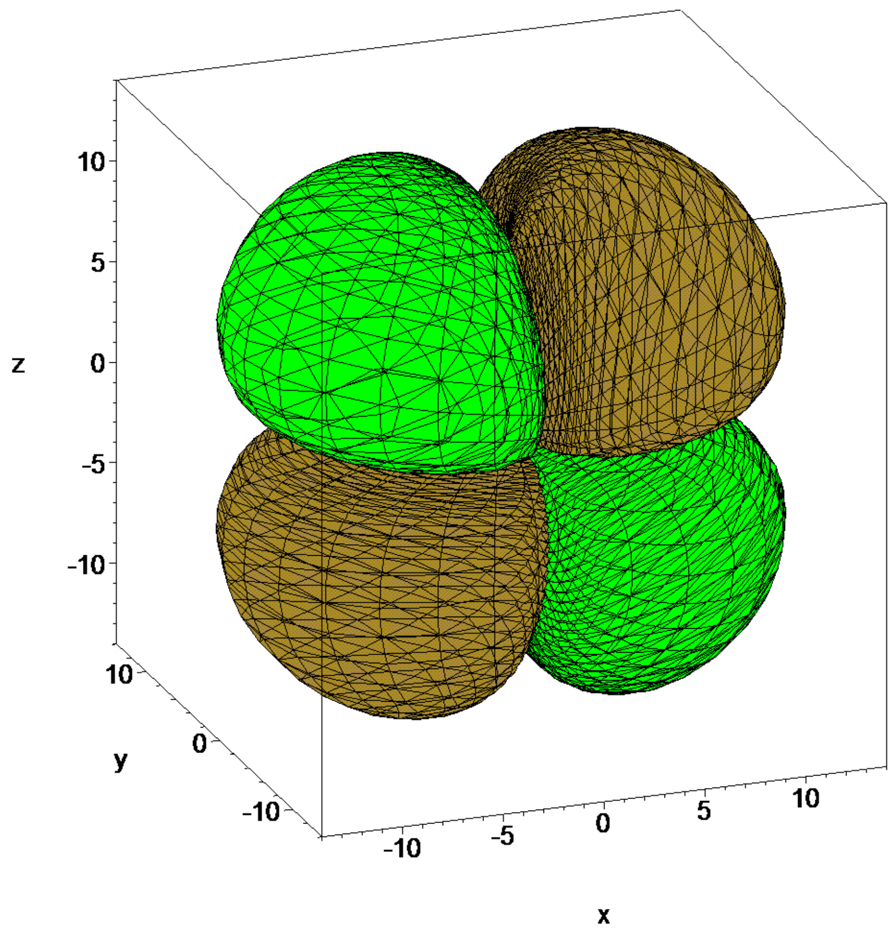


>

and then the surface itself.

```
> plots[implicitplot3d]([eval(ip, cond)=1.45e-6, eval(ip,
  cond)=-1.45e-6], r=0..17,
     theta=0..Pi, phi=0..2*Pi, colour=[sienna, green],
  orientation=[-110,70],
     coords = scispherical, grid=[30,30,30], scaling=constrained,
  axes=box,
     title="amplitude function |2,1,3/2,1/2>, component 4,
  imaginary part",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
  view=[-14..14,-14..14,-14..14]);
```

amplitude function |2,1,3/2,1/2>, component 4, imaginary part



>

The latter two surfaces resemble those of the corresponding real and imaginary parts of $\psi_{0,2,1}(r, \theta, \phi)$. From |2,1,3/2,1/2>,

```
> p := evalc(`|2,1,3/2,1/2>`);
```

$$p := \left[\frac{1}{24}\sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)}\cos(\theta)\right]$$
$$\left[-\frac{1}{48}\sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\phi) - \frac{1}{48} I\sqrt{2}\sqrt{6}\, r\, \mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\sin(\phi)\right]$$

$$\left[\frac{1}{64} I \sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\left(\cos(\theta)^2-\frac{1}{2}\right)\right]$$

$$\left[-\frac{1}{64}\sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\sin(\phi)\right.$$

$$\left.+\frac{1}{64} I \sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\cos(\phi)\right]$$

and its complex conjugate,

```
> pc := evalc(subs(I=-I,`|2,1,3/2,1/2>`));
```

$pc :=$

$$\left[\frac{1}{24}\sqrt{2}\sqrt{6}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\cos(\theta)\right]$$

$$\left[-\frac{1}{48}\sqrt{2}\sqrt{6}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\phi)+\frac{1}{48} I \sqrt{2}\sqrt{6}\,r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\sin(\phi)\right]$$

$$\left[\frac{-1}{64} I \sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\left(\cos(\theta)^2-\frac{1}{2}\right)\right]$$

$$\left[-\frac{1}{64}\sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\sin(\phi)\right.$$

$$\left.-\frac{1}{64} I \sqrt{2}\sqrt{6}\,\alpha Z r\,\mathbf{e}^{\left(-\frac{r}{2}\right)}\sin(\theta)\cos(\theta)\cos(\phi)\right]$$

we form product |2,1,3/2,1/2>* . |2,1,3/2,1/2>,

```
> ps :=
  simplify(evalc(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,3/2,1/2
  >`)) . `|2,1,3/2,1/2>`)) assuming real;
```

$$ps := \frac{1}{12288} r^2\,\mathbf{e}^{(-r)}\left(9 Z^2 \alpha^2+192\cos(\theta)^2+64\right)$$

which we separate into large and small parts.

```
> fl := remove(has, expand(ps), alpha);
```

$$fl := \frac{1}{64}\frac{r^2\cos(\theta)^2}{\mathbf{e}^r}+\frac{1}{192}\frac{r^2}{\mathbf{e}^r}$$

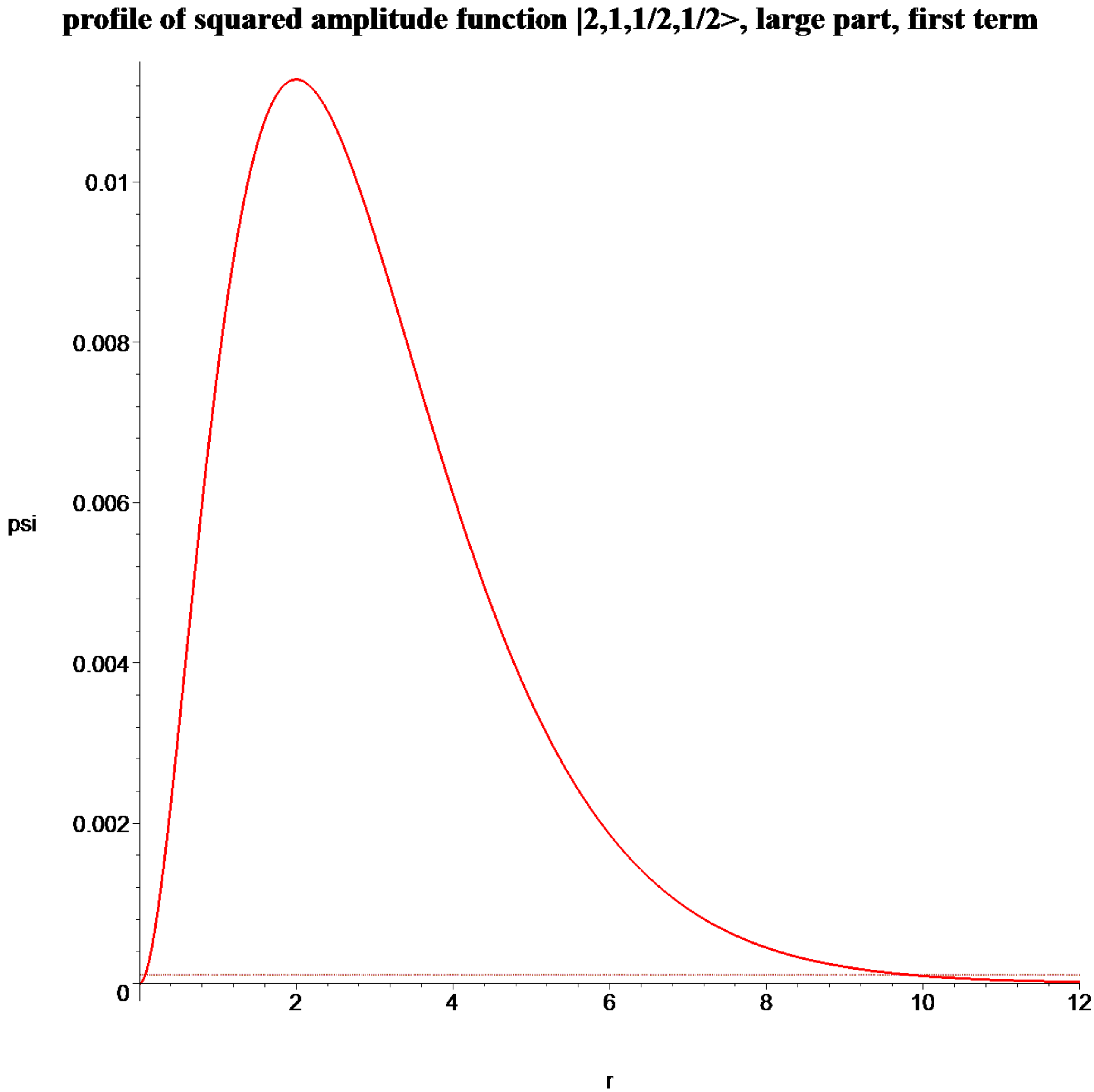
```
> fs := simplify(ps - fl);
```

$$fs := \frac{3}{4096}\mathbf{e}^{(-r)} Z^2 \alpha^2 r^2$$

We plot the radial profile of the large part of squared |2,1,3/2,1/2> that consists of two terms,

```
> plot([eval(fl, [op(cond), theta=0]), 1.14e-4], r=0..12,
```

```
      title="profile of squared amplitude function
|2,1,1/2,1/2>, large part, first term",
      titlefont=[TIMES,BOLD,14], colour=[red, brown, green],
linestyle=[1,2],
      labels=["r", "psi"], thickness=[3,2]);
```



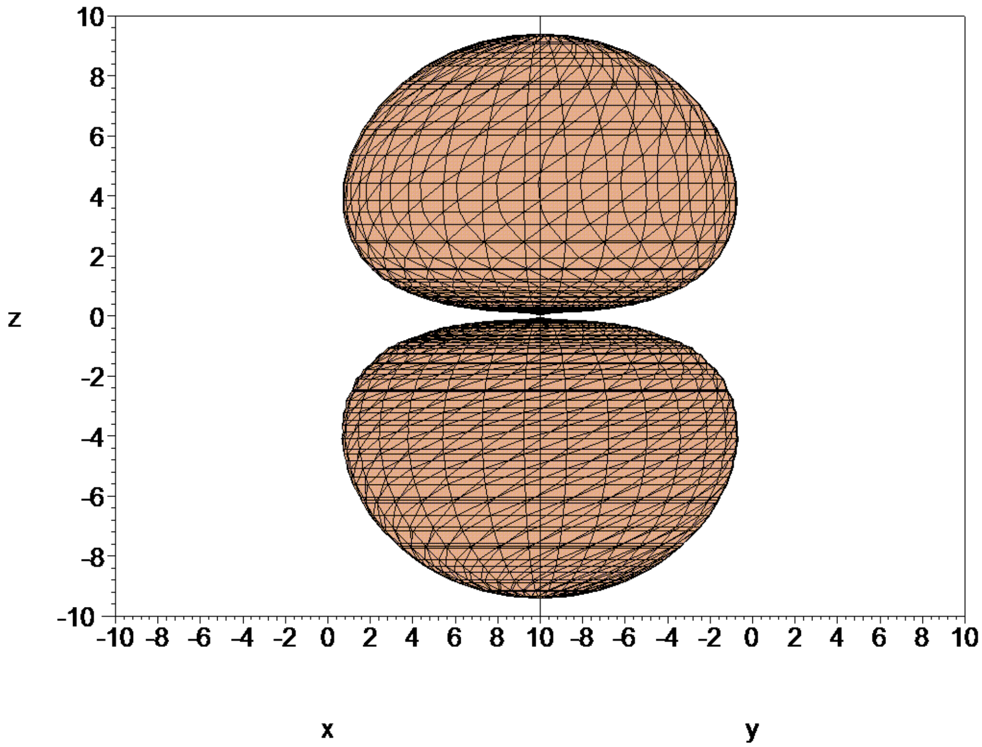
>

the surface of the first term,

```
> plots[implicitplot3d](eval(op(1,fl), cond)=1.14e-4, r=0..13,
  theta=0..Pi, phi=0..2*Pi,
     colour=tan, orientation=[-45,90], labels=["x","y","z"],
  coords = scispherical, axes=box,
     scaling=constrained, title="squared amplitude function
```

```
|2,1,3/2,1/2>, large part, first term",
   grid=[30,30,30], titlefont=[TIMES,BOLD,14],
view=[-10..10,-10..10,-10..10]);
```

squared amplitude function |2,1,3/2,1/2>, large part, first term



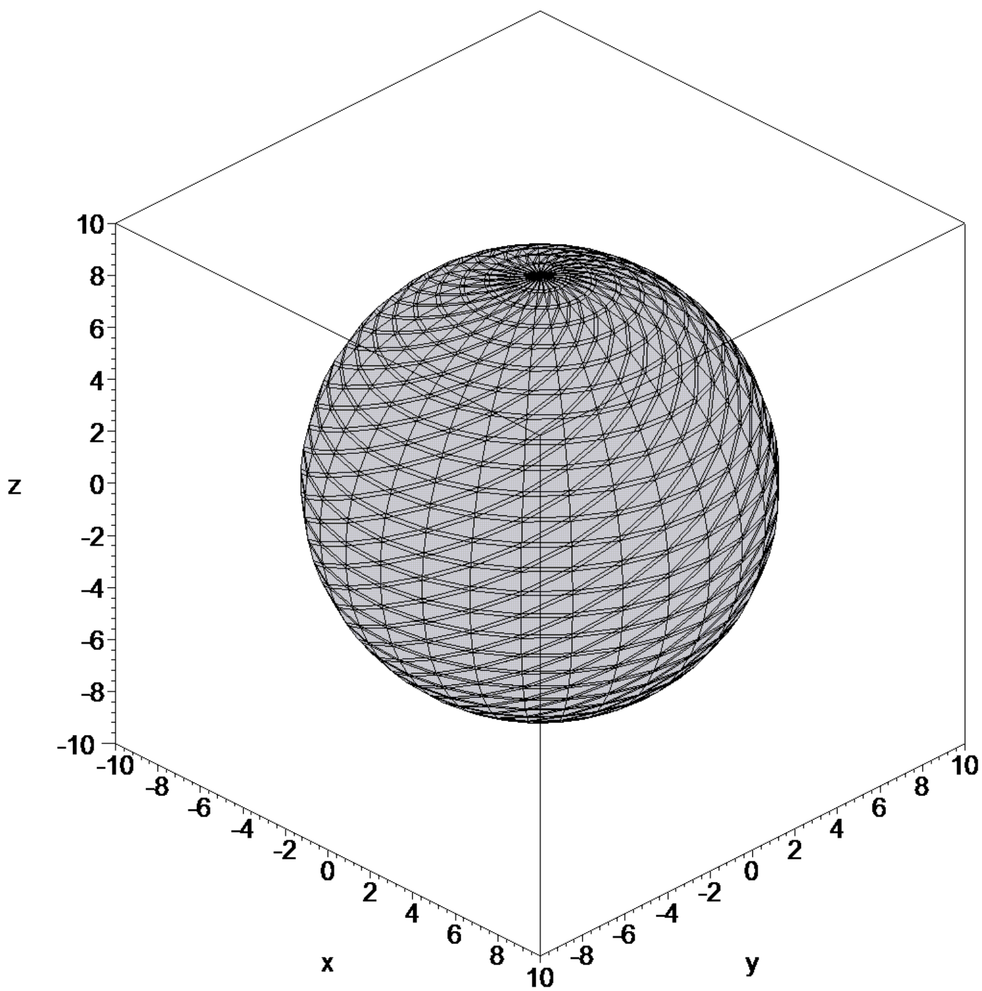

```
>
```

the surface of the second term,

```
> plots[implicitplot3d](eval(op(2,fl), cond)=1.14e-4, r=0..13,
theta=0..Pi, phi=0..2*Pi,
   colour=grey, orientation=[-45,60], labels=["x","y","z"],
coords = scispherical, axes=box,
   scaling=constrained, title="squared amplitude function
|2,1,3/2,1/2>, large part, second term",
   grid=[30,30,30], titlefont=[TIMES,BOLD,14],
```

```
view=[-10..10,-10..10,-10..10]);
```

squared amplitude function |2,1,3/2,1/2>, large part, second term



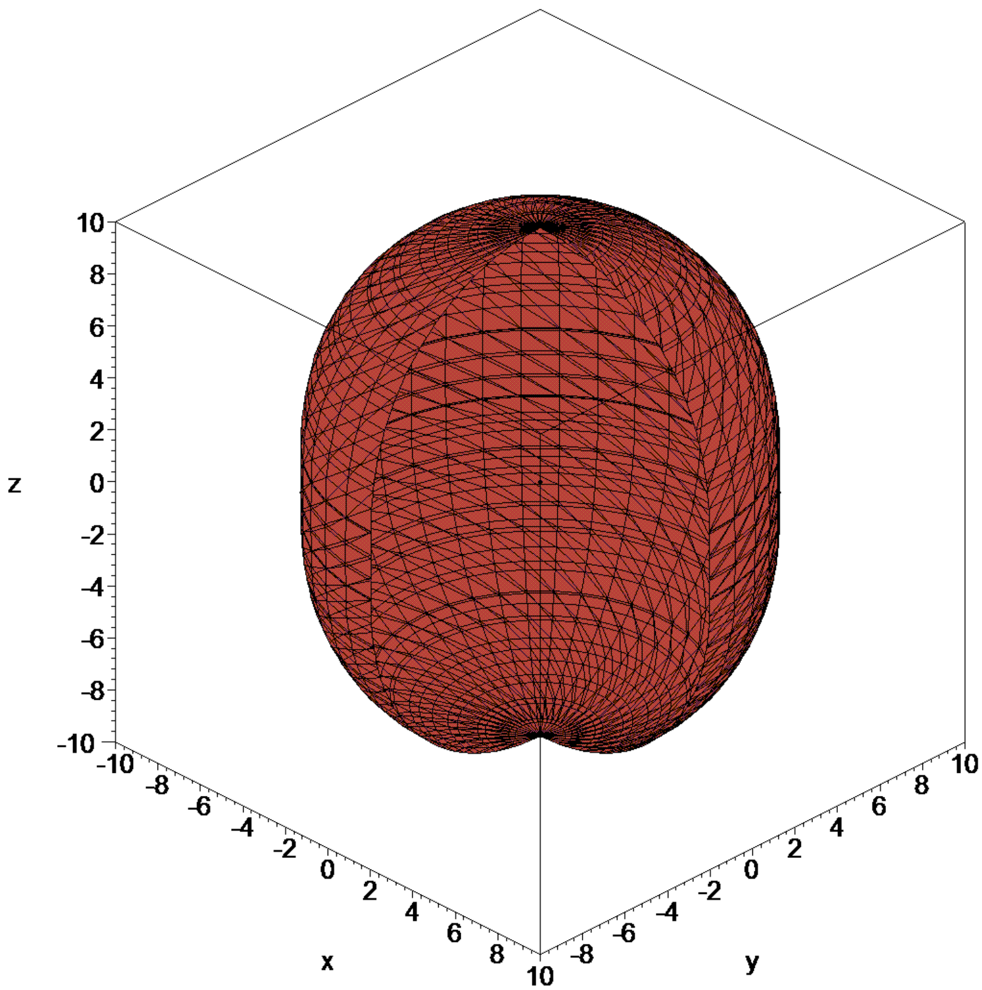
>

of which the first term yields a surface that resembles the surface of $\psi_{0,1,0}(r, \theta, \phi)^2$ whereas the second term yields a surface that resembles that of $\psi_{0,0,0}(r, \theta, \phi)$ or its square; the total large part of squared amplitude function |2,1,3/2,1/2>,

```
> plots[implicitplot3d](eval(fl, cond)=1.14e-4, r=0..13,
  theta=0..Pi, phi=0..3/2*Pi,
     colour=brown, orientation=[-45,60], labels=["x","y","z"],
  coords = scispherical, axes=box,
     scaling=constrained, title="squared amplitude function
  |2,1,3/2,1/2>, total large part",
```

```
    grid=[30,30,30], titlefont=[TIMES,BOLD,14],
  view=[-10..10,-10..10,-10..10]);
```

squared amplitude function |2,1,3/2,1/2>, total large part

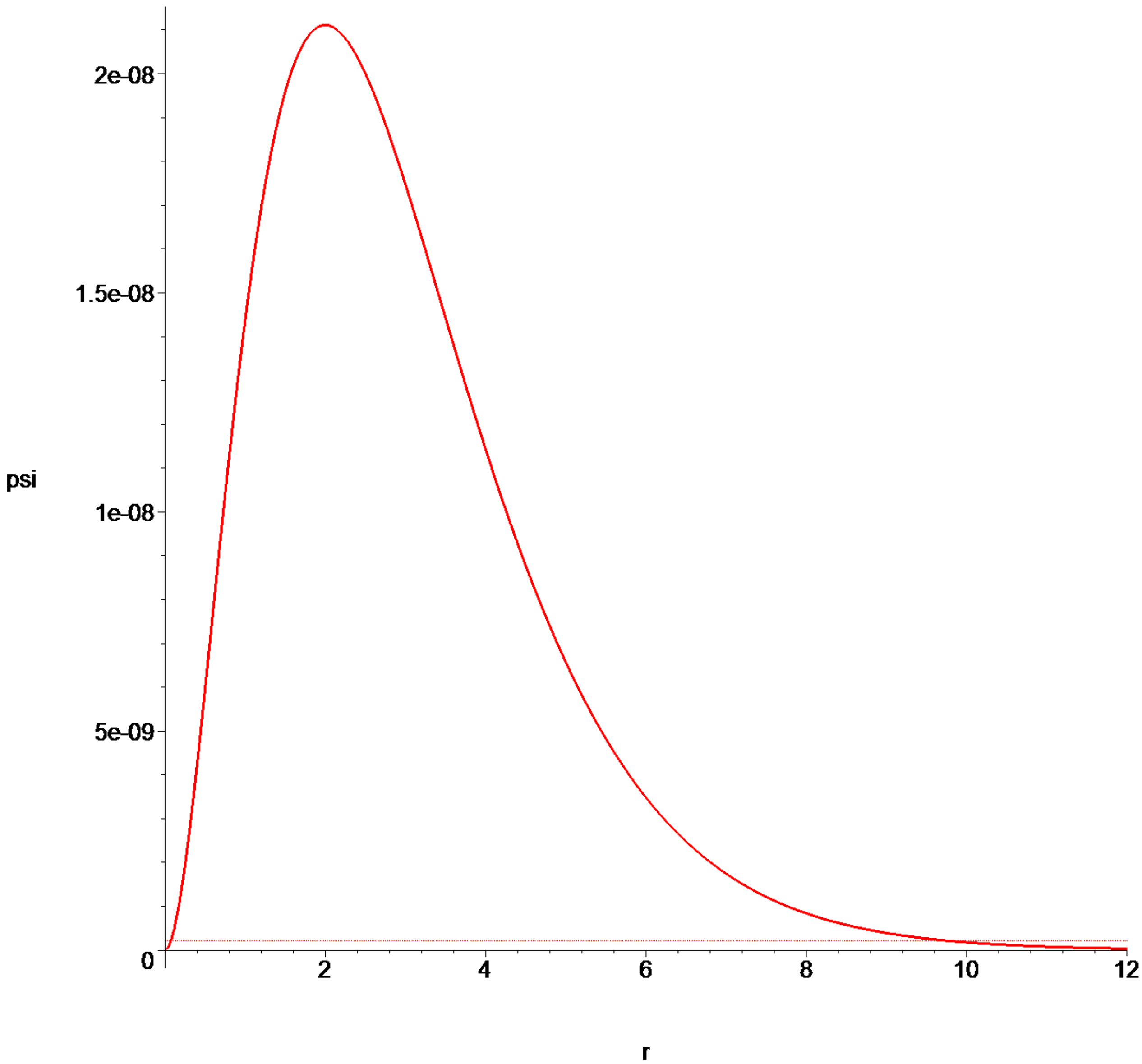


>

which exhibits only one prolate spheroidal lobe symmetric about the polar axis that has no direct counterpart in a single function of $\psi_{k,\,l,\,m}(r,\,\theta,\,\phi)$. We plot the radial profile of the small part of squared amplitude function |2,1,3/2,1/2>,

```
> plot([eval(fs, cond), 2.12e-10], r=0..12,
    title="profile of squared amplitude function |2,1,3/2,1/2>,
  small part",
    titlefont=[TIMES,BOLD,14], colour=[red, brown],
  linestyle=[1,2],
    labels=["r", "psi"], thickness=[3,2]);
```

profile of squared amplitude function |2,1,3/2,1/2>, small part

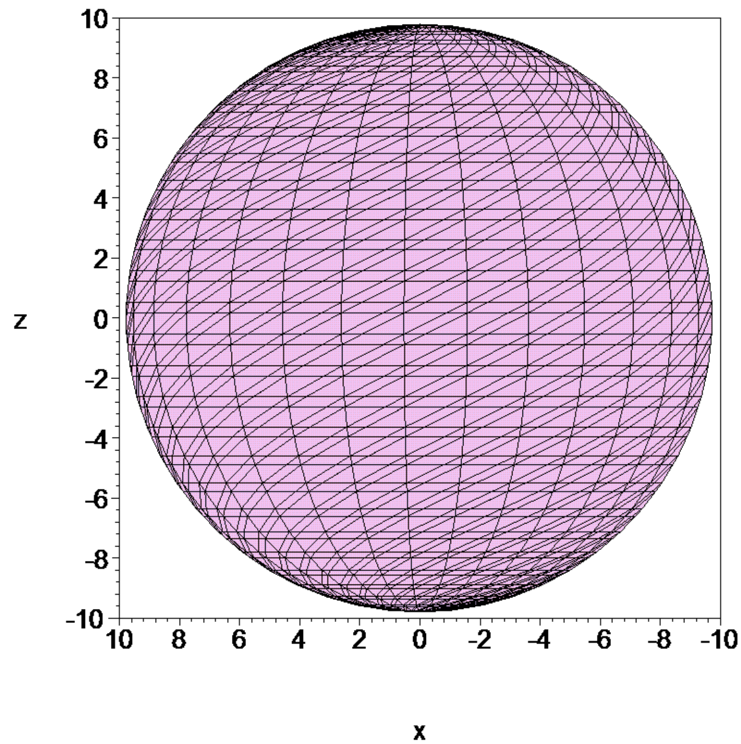


\>

and the surface of the small part of |2,1,3/2,1/2> squared.

```
> plots[implicitplot3d](eval(fs, cond)=2.12e-10, r=0..12,
  theta=0..Pi, phi=0..2*Pi,
     colour=plum, orientation=[90,90],coords = scispherical,
  grid=[30,30,30], axes=box,
     scaling=constrained, title="squared amplitude function
  |2,1,3/2,1/2>, small part",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
  view=[-10..10,-10..10,-10..10]);
```

squared amplitude function |2,1,3/2,1/2>, small part



>

Whereas the large part of squared amplitude function |2,1,3/2,1/2> has both a spherical contribution and a cylindrically symmetric contribution, the surface of the small part of this squared function has only a spherical contribution that resembles the surface of $\psi_{0,0,0}(r, \theta, \phi)$ or its square..

These surfaces of the amplitude functions and their squares show varied shapes similar to those of particular amplitude functions and their squares derived from the solution of the temporally independent Schroedinger equation in spherical polar coordinates, as noted in each case. Some notable features of these surfaces and their underlying formuulae are that, although the small components are either entirely imaginary or complex, the large components are either entirely real or complex; amplitude functions with the same values of j and m have the same angular distribution; the spherically symmetric distribution of amplitude occurs not only with $l = 0$ but also with l =1, for instance for |2,1,1/2,1/2>; toroidal distributions are found for not only the squared amplitude functions but also components of an amplitude function, such as the third component of |2,1,3/2,1/2>; although nodal surfaces exist for the components of the amplitude functions, they fail to persist in the squares of those functions; for even the amplitude functions with $l = 0$, some components have not spherically symmetric surfaces but cylindrically symmetric about the polar axis and the other two axes perpendicular to the polar axis. Other functions -- their components and their large and small parts -- can be analogously plotted.

Apart from the probability density, to which the density of electronic charge is proportional, shown in plots of the surfaces of squared amplitude functions above, a quantum-mechanical problem implies a probability flux; in the stationary state this flux might not vanish, but its divergence must be zero so that probability is locally conserved. In units of c, the spatial components of this probability flux are calculated from $\psi^* \alpha_x \psi$, $\psi^* \alpha_y \psi$ and $\psi^* \alpha_z \psi$, in which velocity matrices α_x, α_y, α_z are the Dirac matrices defined as α1 above in terms of c; ψ is in terms of $\sqrt{\frac{Z^3}{\pi a_0^3}}$. We undertake these calculations, with r in unit $\frac{a_0}{Z}$, for each amplitude function treated above, first for |1,0,1/2,1/2>.

```
> J[x] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|1,0,1/2,1/2>`)) .
  alpha1[x] . `|1,0,1/2,1/2>`);
```

$$J_x := -\alpha Z \mathbf{e}^{(-2r)} \sin(\theta) \sin(\phi)$$

```
> J[y] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|1,0,1/2,1/2>`)) .
  alpha1[y] . `|1,0,1/2,1/2>`);
```

$$J_y := \alpha Z \mathbf{e}^{(-2r)} \sin(\theta) \cos(\phi)$$

```
> J[z] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|1,0,1/2,1/2>`)) .
  alpha1[z] . `|1,0,1/2,1/2>`);
```

$$J_z := 0$$

The magnitude of these components of the probability flux multiplied by the charge on the electron and the speed of light generates this density of circulating electric current.

```
> i := -e*c*simplify(sqrt(J[x]^2 + J[y]^2 + J[z]^2), symbolic)
  assuming real;
```

$$i := -e\, c\, Z \alpha \sin(\theta)\, \mathbf{e}^{(-2r)}$$

We treat similarly |1,0,1/2,-1/2>,

```
> J[x] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|1,0,1/2,-1/2>`))
  . alpha1[x] . `|1,0,1/2,-1/2>`);
```

$$J_x := \alpha Z \mathbf{e}^{(-2r)} \sin(\theta) \sin(\phi)$$

```
> J[y] :=
```

```
simplify(subs(I=-I,LinearAlgebra:-Transpose(`|1,0,1/2,-1/2>`))
. alpha1[y] . `|1,0,1/2,-1/2>`);
```

$$J_y := -\alpha\, Z\, \mathbf{e}^{(-2\, r)} \sin(\theta) \cos(\phi)$$

```
> J[z] :=
simplify(subs(I=-I,LinearAlgebra:-Transpose(`|1,0,1/2,-1/2>`))
. alpha1[z] . `|1,0,1/2,-1/2>`);
```

$$J_z := 0$$

```
> i := -e*c*simplify(sqrt(J[x]^2 + J[y]^2 + J[z]^2), symbolic)
assuming real;
```

$$i := -e\, c\, Z\, \alpha \sin(\theta)\, \mathbf{e}^{(-2\, r)}$$

which yields the same circulating current density as for 1,0,1/2,1/2>.; the signs of J_x and J_y are reversed between these two cases, but because their squares are applied to calculate the current density this effect makes no difference. We treat in the same manner |2,0,1/2,1/2>,

```
> J[x] :=
simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,0,1/2,1/2>`)) .
alpha1[x] . `|2,0,1/2,1/2>`);
```

$$J_x := -\frac{1}{64}\, \alpha\, Z\, (-4 + r)\, \mathbf{e}^{(-r)} \sin(\theta)\, (-2 + r) \sin(\phi)$$

```
> J[y] :=
simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,0,1/2,1/2>`)) .
alpha1[y] . `|2,0,1/2,1/2>`);
```

$$J_y := \frac{1}{64}\, \alpha\, Z\, (-4 + r)\, \mathbf{e}^{(-r)} \sin(\theta)\, (-2 + r) \cos(\phi)$$

```
> J[z] :=
simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,0,1/2,1/2>`)) .
alpha1[z] . `|2,0,1/2,1/2>`);
```

$$J_z := 0$$

```
> i := -e*c*simplify(sqrt(J[x]^2 + J[y]^2 + J[z]^2), symbolic)
assuming real;
```

$$i := -\frac{1}{64}\, e\, c\, \alpha\, Z\, (-4 + r)\, (-2 + r) \sin(\theta)\, \mathbf{e}^{(-r)}$$

and |2,0,1/2,-1/2>,

```
> J[x] :=
simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,0,1/2,-1/2>`))
. alpha1[x] . `|2,0,1/2,-1/2>`);
```

$$J_x := \frac{1}{64}\, \alpha\, Z\, (-4 + r)\, \mathbf{e}^{(-r)} \sin(\theta)\, (-2 + r) \sin(\phi)$$

```
> J[y] :=
simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,0,1/2,-1/2>`))
```

```
. alpha1[y] . `|2,0,1/2,-1/2>`);
```

$$J_y := -\frac{1}{64}\alpha Z(-4+r)\mathbf{e}^{(-r)}\sin(\theta)(-2+r)\cos(\phi)$$

```
> J[z] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,0,1/2,-1/2>`))
  . alpha1[z] . `|2,0,1/2,-1/2>`);
```

$$J_z := 0$$

```
> i := -e*c*simplify(sqrt(J[x]^2 + J[y]^2 + J[z]^2), symbolic)
  assuming real;
```

$$i := -\frac{1}{64}e\,c\,\alpha Z(-4+r)(-2+r)\sin(\theta)\mathbf{e}^{(-r)}$$

|2,1,1/2,1/2>,

```
> J[x] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,1/2,1/2>`)) .
  alpha1[x] . `|2,1,1/2,1/2>`);
```

$$J_x := \frac{1}{192}\alpha Z(-6+r)\mathbf{e}^{(-r)}r\sin(\theta)\sin(\phi)$$

```
> J[y] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,1/2,1/2>`)) .
  alpha1[y] . `|2,1,1/2,1/2>`);
```

$$J_y := -\frac{1}{192}\alpha Z(-6+r)\mathbf{e}^{(-r)}r\sin(\theta)\cos(\phi)$$

```
> J[z] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,1/2,1/2>`)) .
  alpha1[z] . `|2,1,1/2,1/2>`);
```

$$J_z := 0$$

```
> i := -e*c*simplify(sqrt(J[x]^2 + J[y]^2 + J[z]^2), symbolic)
  assuming real;
```

$$i := -\frac{1}{192}e\,c\,\alpha Z(-6+r)r\sin(\theta)\mathbf{e}^{(-r)}$$

|2,1,1/2,-1/2>,

```
> J[x] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,1/2,-1/2>`))
  . alpha1[x] . `|2,1,1/2,-1/2>`);
```

$$J_x := \frac{1}{192}\alpha Z(-6+r)\mathbf{e}^{(-r)}r\sin(\theta)\sin(\phi)$$

```
> J[y] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,1/2,-1/2>`))
  . alpha1[y] . `|2,1,1/2,-1/2>`);
```

$$J_y := -\frac{1}{192}\,\alpha\,Z\,(-6+r)\,\mathbf{e}^{(-r)}\,r\sin(\theta)\cos(\phi)$$

```
> J[z] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,1/2,-1/2>`))
  . alpha1[z] . `|2,1,1/2,-1/2>`);
```

$$J_z := 0$$

```
> i := -e*c*simplify(sqrt(J[x]^2 + J[y]^2 + J[z]^2), symbolic)
  assuming real;
```

$$i := -\frac{1}{192}\,e\,c\,\alpha\,Z\,(-6+r)\,r\sin(\theta)\,\mathbf{e}^{(-r)}$$

|2,1,3/2,3/2>,

```
> J[x] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,3/2,3/2>`)) .
  alpha1[x] . `|2,1,3/2,3/2>`);
```

$$J_x := -\frac{1}{128}\,\alpha\,Z\,r^2\,\mathbf{e}^{(-r)}\sin(\theta)^3\sin(\phi)$$

```
> J[y] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,3/2,3/2>`)) .
  alpha1[y] . `|2,1,3/2,3/2>`);
```

$$J_y := \frac{1}{128}\,\alpha\,Z\,r^2\,\mathbf{e}^{(-r)}\sin(\theta)^3\cos(\phi)$$

```
> J[z] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,3/2,3/2>`)) .
  alpha1[z] . `|2,1,3/2,3/2>`);
```

$$J_z := 0$$

```
> i := -e*c*simplify(sqrt(J[x]^2+J[y]^2+J[z]^2), symbolic)
  assuming real:
  i := simplify(subs(cos(theta)^2 = 1 -  sin(theta)^2, i),
  symbolic);
```

$$i := -\frac{1}{128}\,e\,c\,r^2\,\alpha\,Z\,\mathbf{e}^{(-r)}\sin(\theta)^3$$

and |2,1,3/2,1/2>.

```
> J[x] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,3/2,1/2>`)) .
  alpha1[x] . `|2,1,3/2,1/2>`);
```

$$J_x := -\frac{3}{128}\sin(\theta)\,\mathbf{e}^{(-r)}\,Z\left(\cos(\theta)^2-\frac{1}{6}\right)\sin(\phi)\,\alpha\,r^2$$

```
> J[y] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,3/2,1/2>`)) .
  alpha1[y] . `|2,1,3/2,1/2>`);
```

$$J_y := \frac{1}{256}\,\alpha\, Z\, r^2\, \mathbf{e}^{(-r)} \sin(\theta)\,(6\cos(\theta)^2 - 1)\cos(\phi)$$

```
> J[z] :=
  simplify(subs(I=-I,LinearAlgebra:-Transpose(`|2,1,3/2,1/2>`)) .
  alpha1[z] . `|2,1,3/2,1/2>`);
```

$$J_z := 0$$

```
> i := -e*c*simplify(sqrt(J[x]^2+J[y]^2+J[z]^2), symbolic)
  assuming real;
```

$$i := -\frac{1}{256}\, e\, c\, r^2 \sin(\theta)\,(6\cos(\theta)^2 - 1)\, Z\, \alpha\, \mathbf{e}^{(-r)}$$

In each case, summarised in the following table in SI units and incorporating Bohr radius a_0 with all pertinent factors, there is a finite electric current density that circulates about the polar axis, which differs for each amplitude function but is largest for the amplitude function for the hydrogen atom (with $Z = 1$) in its ground electronic state; there is no current density parallel to this axis as each current density is proportional to $\sin(\theta)$ to some power.

function or state	magnitude of circulating current
|1,0,1/2,±1/2>	$-\frac{e\, c\, \alpha\, Z^4 \sin(\theta)\, \mathbf{e}^{\left(-\frac{2 Z r}{a_0}\right)}}{\pi\, a_0^{\,3}}$
|2,0,1/2,±1/2>	$-\frac{e\, c\, \alpha\, Z^4 \left(-4 + \frac{Z r}{a_0}\right)\left(\frac{Z r}{a_0} - 2\right) \sin(\theta)\, \mathbf{e}^{\left(-\frac{Z r}{a_0}\right)}}{64\, \pi\, a_0^{\,3}}$
|2,1,1/2,±1/2>	$-\frac{e\, c\, \alpha\, Z^5 \left(-6 + \frac{Z r}{a_0}\right) r \sin(\theta)\, \mathbf{e}^{\left(-\frac{Z r}{a_0}\right)}}{192\, \pi\, a_0^{\,4}}$
|2,1,3/2,±3/2>	$-\frac{e\, c\, \alpha\, Z^6\, r^2\, \mathbf{e}^{\left(-\frac{Z r}{a_0}\right)} \sin(\theta)^3}{128\, \pi\, a_0^{\,5}}$
|2,1,3/2,±1/2>	$-\frac{e\, c\, \alpha\, Z^6\, r^2 \sin(\theta)\,(6\cos(\theta)^2 - 1)\, \mathbf{e}^{\left(-\frac{Z r}{a_0}\right)}}{256\, \pi\, a_0^{\,5}}$

The two signs + and - of the square root in the calculation of current i allow for the opposite directions of flow for $m = \frac{1}{2}$ or $m = -\frac{1}{2}$ for instance, but there is no correlation between that sign of the square root and the sign of m. For ground state $|1,0,1/2,\pm 1/2>$, the magnitude of the circulating current of electric charge is

$$i = e \int \mathrm{J}(r,\theta) \,.\, dS \;=\; e \int_0^{\infty}\int_0^{\pi} J_{\phi}\, r\, d\theta\, dr \;=\; \frac{Z^2\,\alpha\, c\, e}{2\,\pi\, a_0}$$

which is identical with the result of the Bohr-Sommerfeld treatment in section 12b.51 to order α. For the corresponding magnetic dipolar moment, we first write

$$\mathrm{d}\mu \;=\pi\,(r\sin(\theta))^2\,\mathrm{d}i \;=\; \pi\, r^3 \sin(\theta)^2\, e\, J_{\phi}\, \mathrm{d}r\, \mathrm{d}\theta$$

so to obtain

$$\mu = \frac{Z^4\,\alpha\, c\, e}{a_0^{\,3}} \int_0^{\pi} \sin(\theta)^3\, d\theta \int_0^{\infty} \mathbf{e}^{\left(-\frac{2\,Z\,e}{a_0}\right)} r^3\, dr \;=\; \frac{1}{2}\,\alpha\, c\, a_0\, e$$

again in accord with the result from Bohr and Sommerfeld for n = 1, l = 0 in section 12b.51. This circulating current density, which depends on r and θ but is independent of equatorial angle ϕ, hence generates a magnetic dipolar moment; the significance of this result is that the circulating current entirely accounts for the magnetic properties associated with the electron in the hydrogen atom, not requiring the postulation of an electron rotating about its axis. For a general state with $|n,l,j,m>$, the magnetic dipolar moment is $\mu \;=\; \dfrac{e\, c\,\alpha\, a_0}{2}\,\dfrac{j+\frac{1}{2}}{l+\frac{1}{2}}\, m$, in which the first part is just the Bohr magneton, the second part is the Lande splitting factor and m is the magnetic quantum number; this formula gives correctly all the magnetic levels of the electron in the hydrogen atom, so that the circulating current is exactly enough to account for all magnetic properties of an electron in the hydrogen atom.

W. Gordon, who with C. G. Darwin first solved the Dirac equation in detail for hydrogen, verified that the Dirac solution for the fine structure was in accord with Sommerfeld to order $Z\,\alpha$. For experimental purposes at the time, Sommerfeld's relativistic generalisation of Bohr's treatment sufficed completely to account for the H fine structure. For this reason, the above two results above for the circulating current and the magnetic dipolar moment might perhaps not astonish - except for the fact that the two descriptions appear to differ so radically. In contrast, according to Schroedinger's formulation in spherical polar coordinates as presented in example *x12b.52*, the contributions to the density of circulating current are $J_r = J_{\theta} = 0$, but $J_{\phi} = -\dfrac{e\, h\, m}{2\,\pi\,\mu\, r\sin(\theta)}\,|\,\psi_{k,\,l,\,m}|^2$, so the current density is non-zero only for equatorial quantum number $m \neq 0$.

There might appear to arise an inconsistency,within the above calculations, in the use of velocity matrices designated with cartesian coordinates and amplitude functions ψ containing spherical polar coordinates in the above products, but when one converts the latter amplitude functions to cartesian form, as presented in section 12b.57 the results are the same, because the velocity matrices contain no explicit cartesian component. An alternative decomposition of the α matrices follows, kindly provided by Professor J. D. Hey.

We express the α matrices in vector notation:

$$\bar{\alpha} = \alpha_x \bar{x} + \alpha_y \bar{y} + \alpha_z \bar{z} \equiv \alpha_r \bar{r} + \alpha_\theta \bar{\theta} + \alpha_\phi \bar{\phi}$$

in which $\bar{x}$, $\bar{y}$, $\bar{z}$, $\bar{r}$, $\bar{\theta}$ and $\bar{\phi}$ are unit vectors corresponding to the coordinates in cartesian and spherical polar systems. For the transformation between systems of coordinates we have

$$\bar{x} = \cos(\phi)\,(\sin(\theta)\,\bar{r} + \cos(\theta)\,\bar{\theta}) - \sin(\phi)\,\bar{\phi},$$

$$\bar{y} = \sin(\phi)\,(\sin(\theta)\,\bar{r} + \cos(\theta)\,\bar{\theta}) + \cos(\phi)\,\bar{\phi} \text{ and}$$

$$\bar{z} = \cos(\theta)\,\bar{r} - \sin(\theta)\,\bar{\theta},$$

we obtain

$$\alpha_r = \sin(\theta)\cos(\phi)\,\alpha_x + \sin(\theta)\sin(\phi)\,\alpha_y + \cos(\theta)\,\alpha_z,$$

$$\alpha_\theta = \cos(\theta)\cos(\phi)\,\alpha_x + \cos(\theta)\sin(\phi)\,\alpha_y - \sin(\theta)\,\alpha_z \text{ and}$$

$$\alpha_\phi = -\sin(\phi)\,\alpha_x + \cos(\phi)\,\alpha_y.$$

In terms of circulating flux, we hence obtain

$$J_r = \psi^*\,\alpha(r)\,\psi = \sin(\theta)\cos(\phi)\,J_x + \sin(\theta)\sin(\phi)\,J_y + \cos(\theta)\,J_z,$$

$$J_\theta = \psi^*\,\alpha_\theta\,\psi = \cos(\theta)\cos(\phi)\,J_x + \cos(\theta)\sin(\phi)\,J_y - \sin(\theta)\,J_z \text{ and}$$

$$J_\phi = \psi^*\,\alpha_\phi\,\psi = -\sin(\phi)\,J_x + \cos(\phi)\,J_y\,.$$

On substitution from equations above for ground state |1,0,1/2,1/2>, we find $J_r = 0$, $J_\theta = 0$ and J_ϕ leads to $i = -\dfrac{e\,Z^4\,\alpha\,c\,\mathbf{e}^{\left(-\frac{2\,Z\,r}{a_0}\right)}}{\pi\,a_0^{\,3}}\sin(\theta)$, consistent with the result above.

We plot in each case these current densities, first the profile at $\theta = \frac{\pi}{2}$, and then the surface.

```
> cond := [e=1,c=1/alpha,Z=1,a[0]=1];
```

$$cond := \left[e = 1,\, c = \frac{1}{\alpha},\, Z = 1,\, a_0 = 1\right]$$

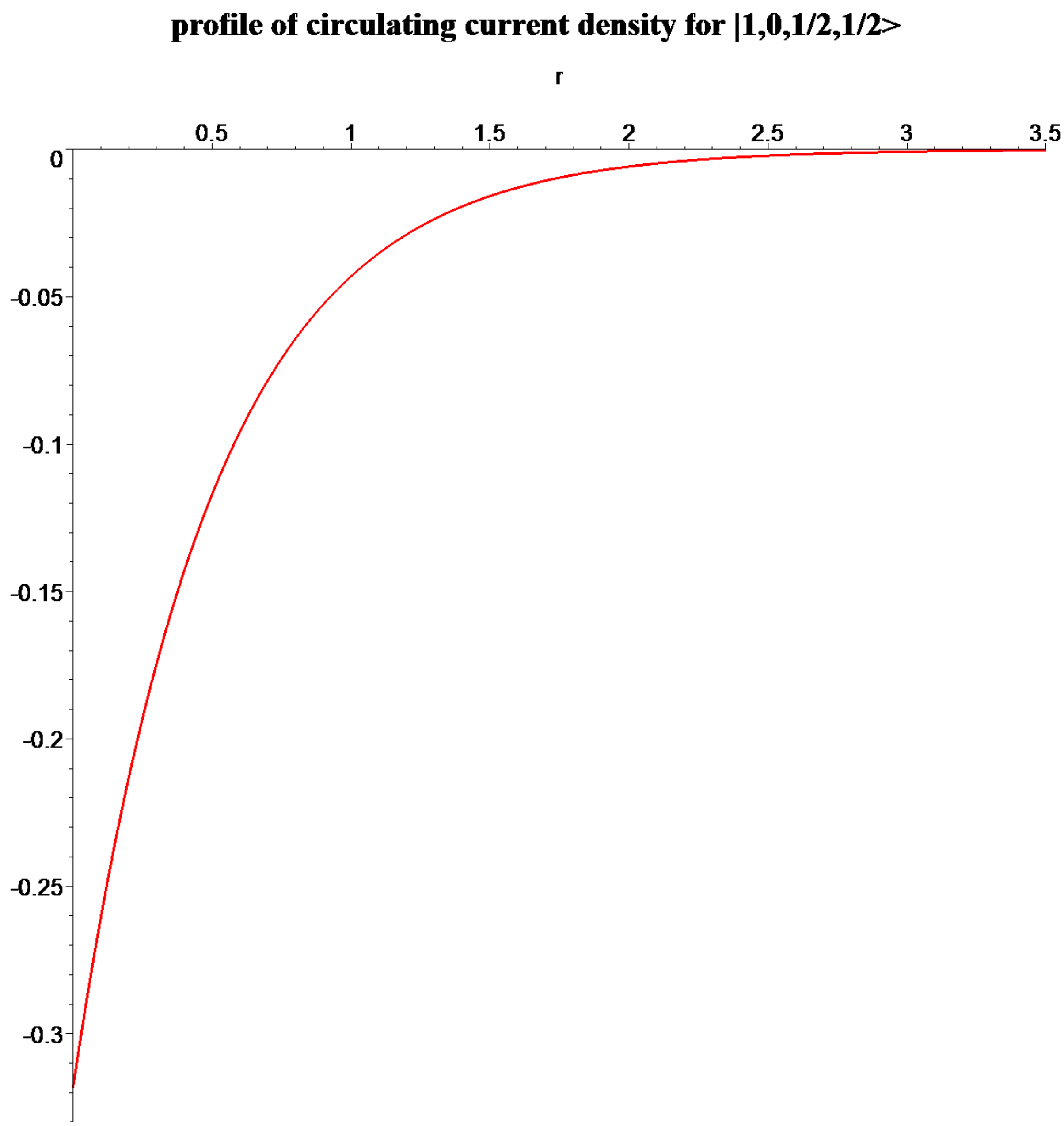
The circulating current density for |1,0,1/2,1/2> or |1,0,1/2,-1/2> has this formula,

```
> cc1 := -e*c*alpha*Z^4*sin(theta)*exp(-2*Z*r/a[0])/(Pi*a[0]^3);
```

$$cc1 := -\frac{e\,c\,\alpha\,Z^4\sin(\theta)\,\mathbf{e}^{\left(-\frac{2\,Z\,r}{a_0}\right)}}{\pi\,a_0^{\,3}}$$

of which we plot the profile of the geometric content with distance in unit of a_0.

```
> plot(eval(cc1, [op(cond),theta=Pi/2]), r=0..3.5, -0.33..0,
  colour=red, titlefont=[TIMES,BOLD,14],
      title="profile of circulating current density for
  |1,0,1/2,1/2>", thickness=3);
```



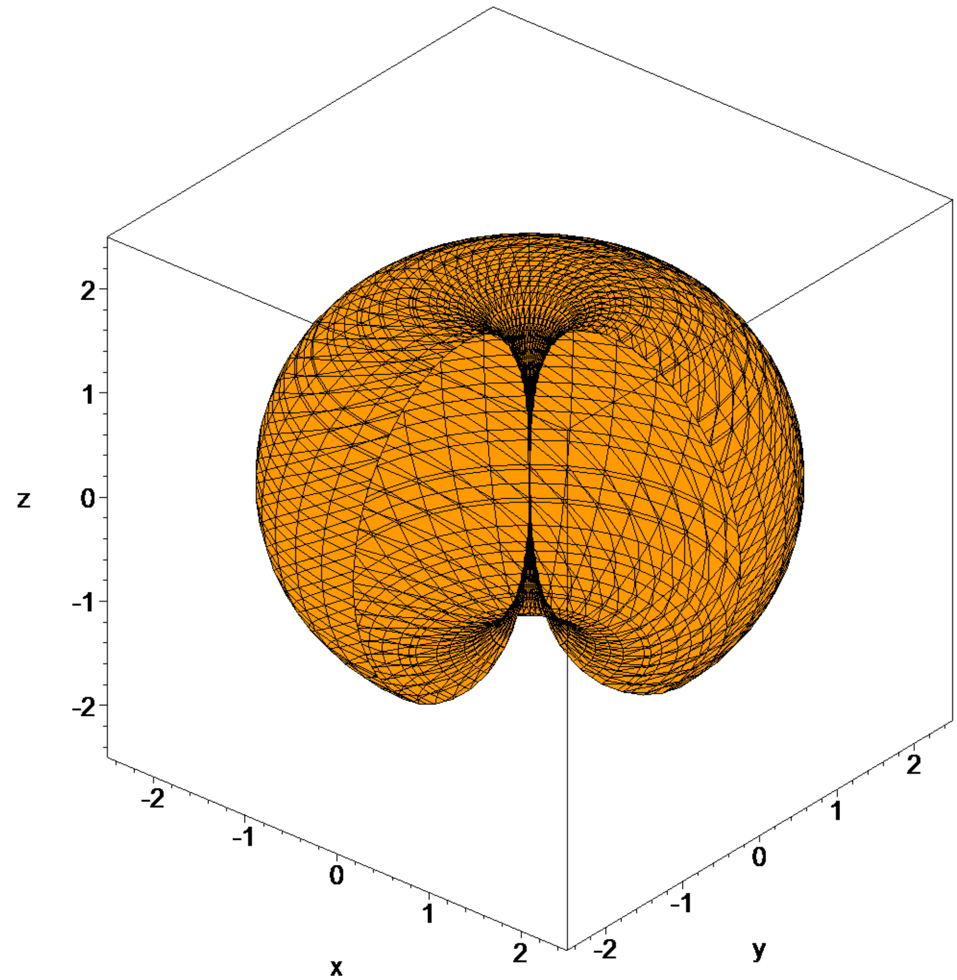
>

Here is the resulting surface of constant circulating current density at $\frac{1}{100}$ of the maximum current density, such that about 0.995 of the total circulating current flows within the surface, which is cut oper to show the internal detail.

```
> plots[implicitplot3d](eval(cc1, cond)=-0.0033, r=0..4,
  theta=0..Pi, phi=0..3/2*Pi,
     colour=coral, orientation=[-50,60],coords = scispherical,
  grid=[30,30,30], axes=box,
     scaling=constrained, title="circulating current density
  |1,0,1/2,1/2>",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
```

```
view=[-2.5..2.5,-2.5..2.5,-2.5..2.5]);
```

circulating current density |1,0,1/2,1/2>



>

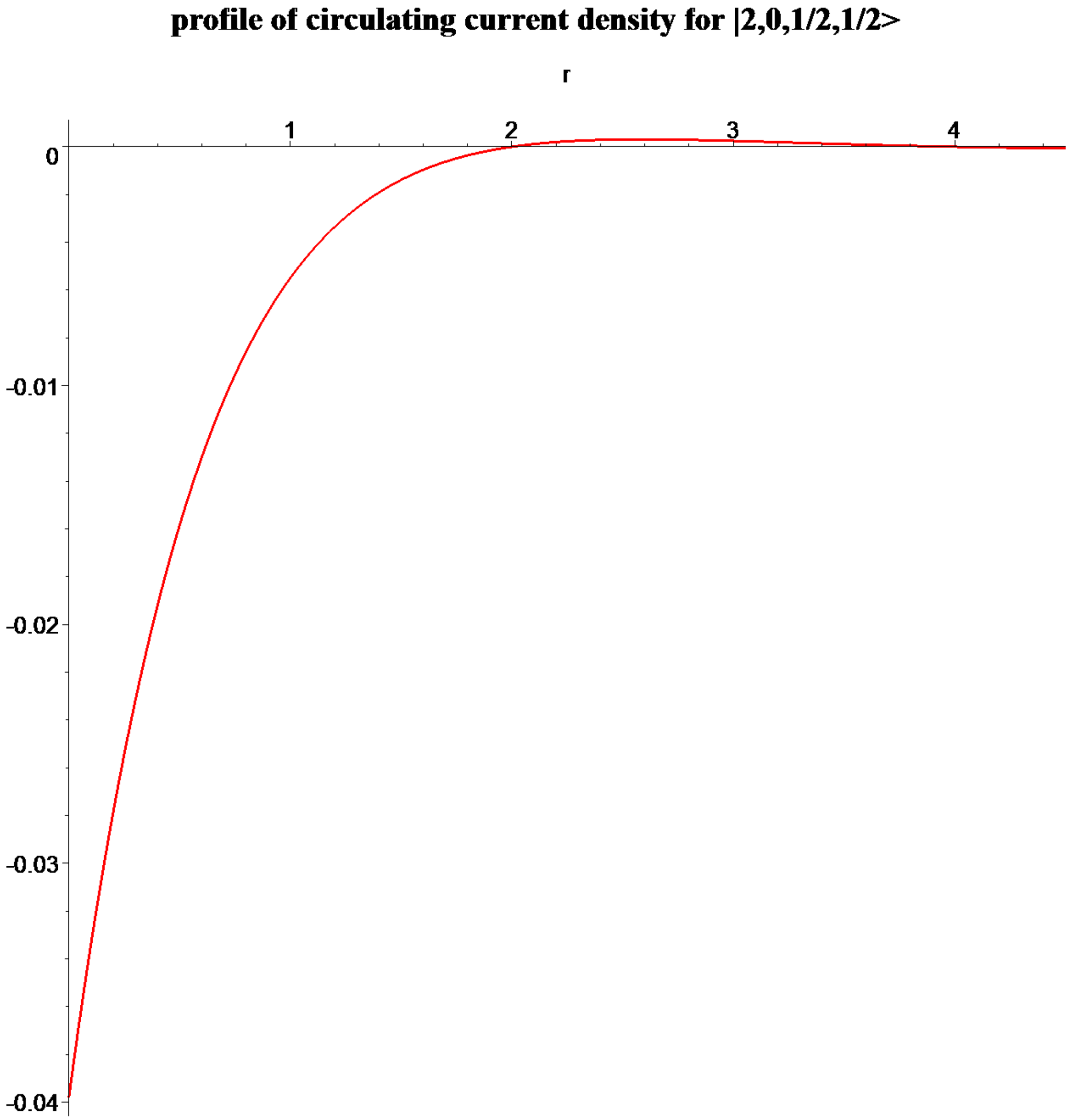
We proceed to }2,0,1/2,1/2>,

```
> cc2 :=
-e*c*alpha*Z^4*(-4+Z*r/a[0])*(Z*r/a[0]-2)*sin(theta)*exp(-Z*r/a
[0])/64/(Pi*a[0]^3);
```

$$cc2 := -\frac{1}{64}\,\frac{e\,c\,\alpha\,Z^4\left(-4+\frac{Z\,r}{a_0}\right)\left(\frac{Z\,r}{a_0}-2\right)\sin(\theta)\,\mathbf{e}^{\left(-\frac{Z\,r}{a_0}\right)}}{\pi\,a_0^{\;3}}$$

with this profile at $\theta = \frac{\pi}{2}$.

```
> plot(eval(cc2, [op(cond),theta=Pi/2]), r=0..4.5, colour=red,
  titlefont=[TIMES,BOLD,14],
          title="profile of circulating current density for
  |2,0,1/2,1/2>", thickness=3);
```

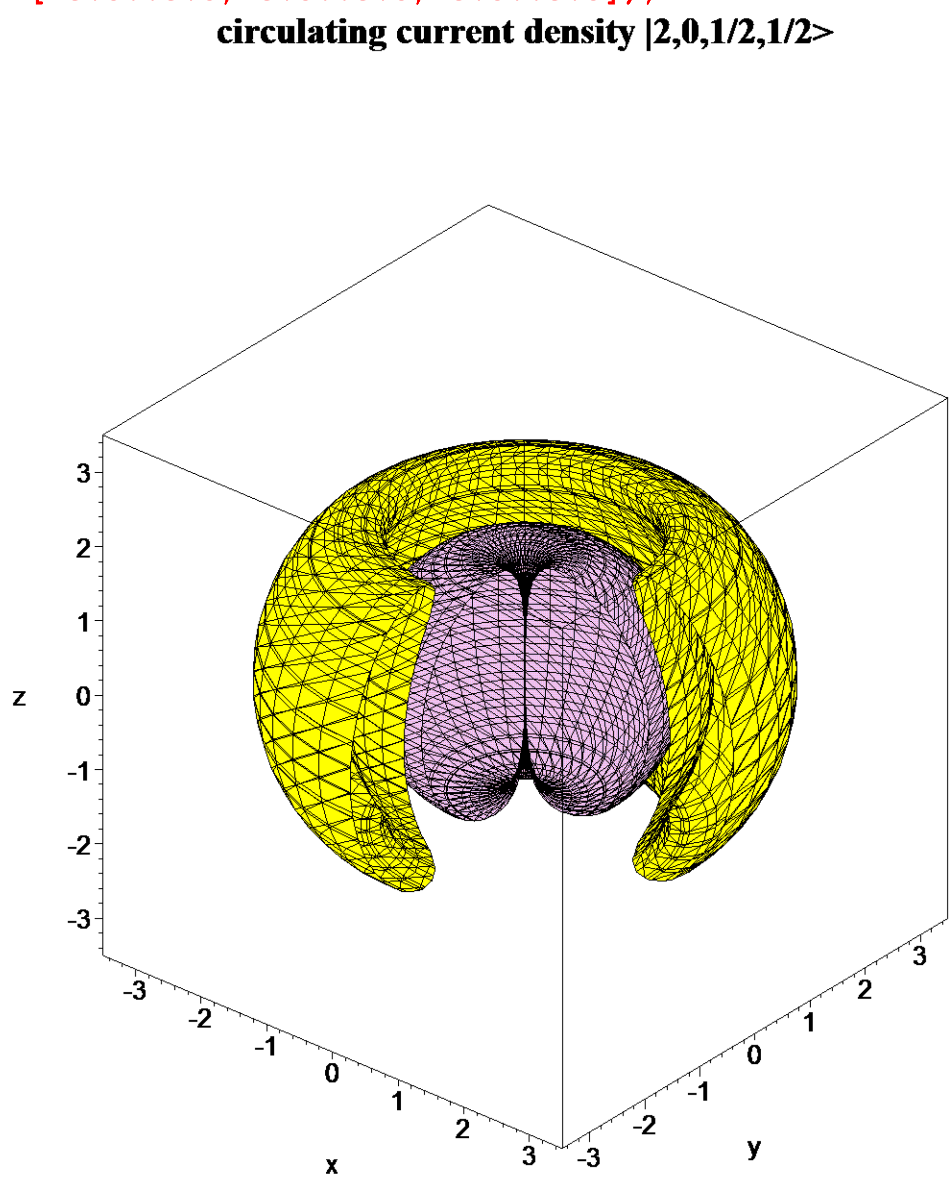



```
>
```

In this case the current flows in opposite directions near and farther from the atomic nucleus on either side of $r = 2\ a_0$, indicated with contrasting colours.

```
> plots[implicitplot3d]([eval(cc2, cond)=-0.0002, eval(cc2,
  cond)=0.0002],
     r=0..4, theta=0..Pi, phi=0..3/2*Pi, colour=[plum,yellow],
```

```
labels=["x","y","z"],
   coords = scispherical, grid=[30,30,30],
orientation=[-50,60], axes=box,
   scaling=constrained, title="circulating current density
|2,0,1/2,1/2>",
   titlefont=[TIMES,BOLD,14],
view=[-3.5..3.5,-3.5..3.5,-3.5..3.5]);
```



\>

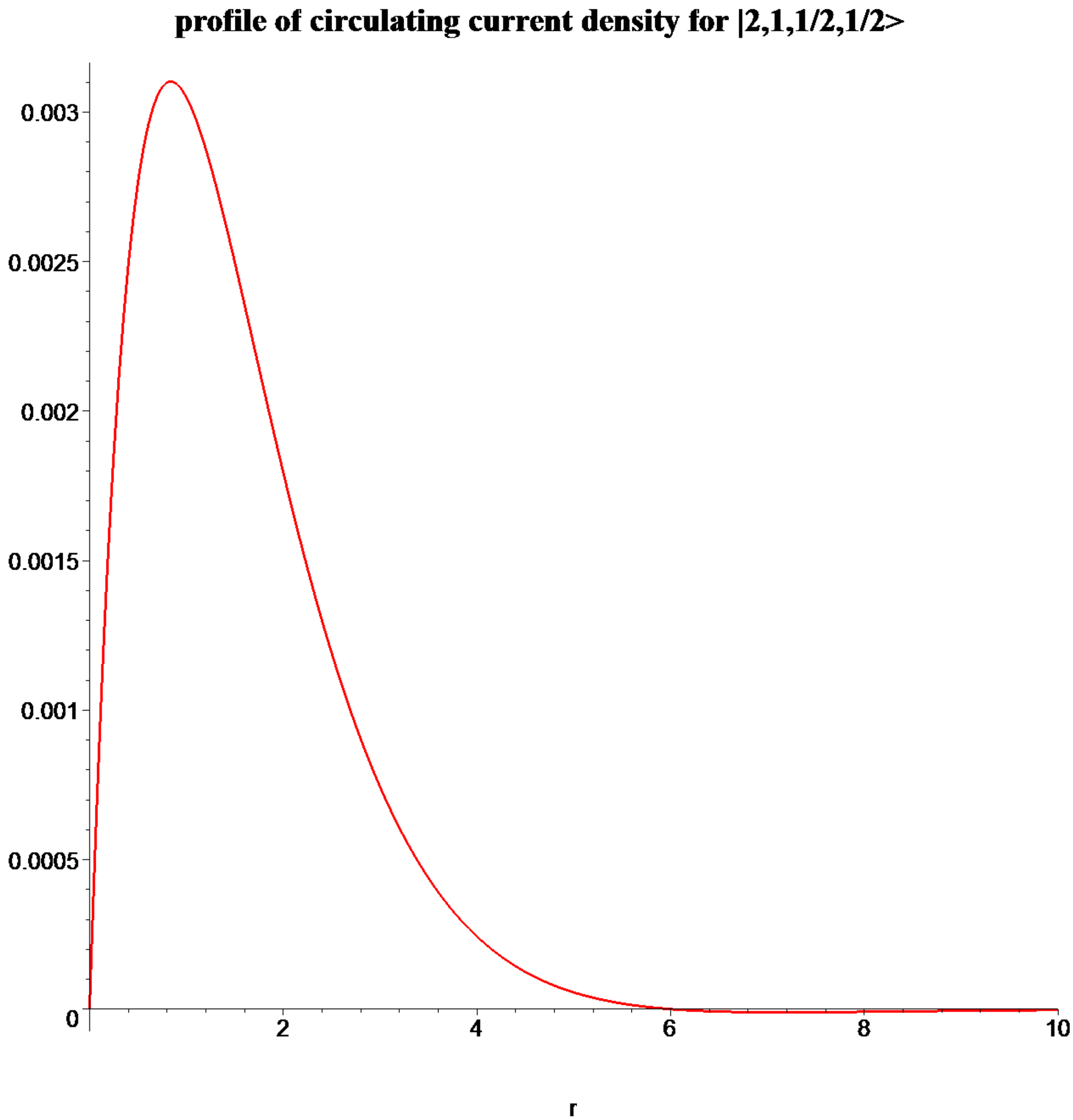
For |2,1,1/2,1/2> we proceed analogously.

```
> cc3 :=
  -e*c*alpha*Z^5*(-6+Z*r/a[0])*r*sin(theta)*exp(-Z*r/a[0])/(192*P
  i*a[0]^4);
```

$$cc3 := -\frac{1}{192}\,\frac{e\,c\,\alpha\,Z^5\left(-6+\frac{Z\,r}{a_0}\right)r\sin(\theta)\,\mathbf{e}^{\left(-\frac{Z\,r}{a_0}\right)}}{\pi\,a_0^{\;4}}$$

Its profile,

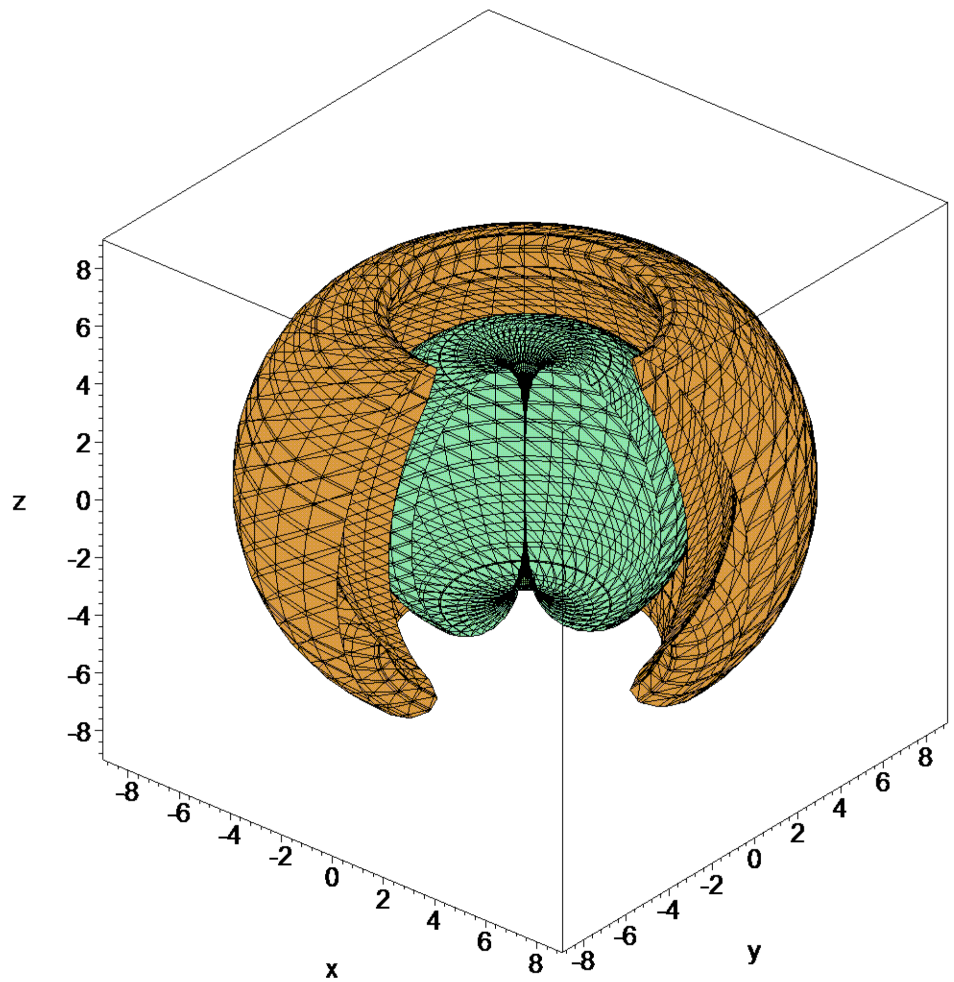
```
> plot(eval(cc3, [op(cond),theta=Pi/2]), r=0..10, colour=red,
  titlefont=[TIMES,BOLD,14],
          title="profile of circulating current density for
  |2,1,1/2,1/2>", thickness=3);
```



>

again shows a reversal of direction of the circulating current, near $r = 6\,a_0$; to show clearly the regions, we amplify the current in the region shown as negative in the profile.

```
> plots[implicitplot3d]([eval(cc3, cond)=0.000031, eval(cc3,
  cond)*5=-0.000031], r=0..12,
     theta=0..Pi, phi=0..3/2*Pi, colour=[aquamarine,gold],
  orientation=[-50,60],
     coords = scispherical, grid=[30,30,30], axes=box,
  scaling=constrained,
     labels=["x","y","z"], #title="circulating current density
  |2,1,1/2,1/2>",
     titlefont=[TIMES,BOLD,14], view=[-9..9,-9..9,-9..9]);
```



>

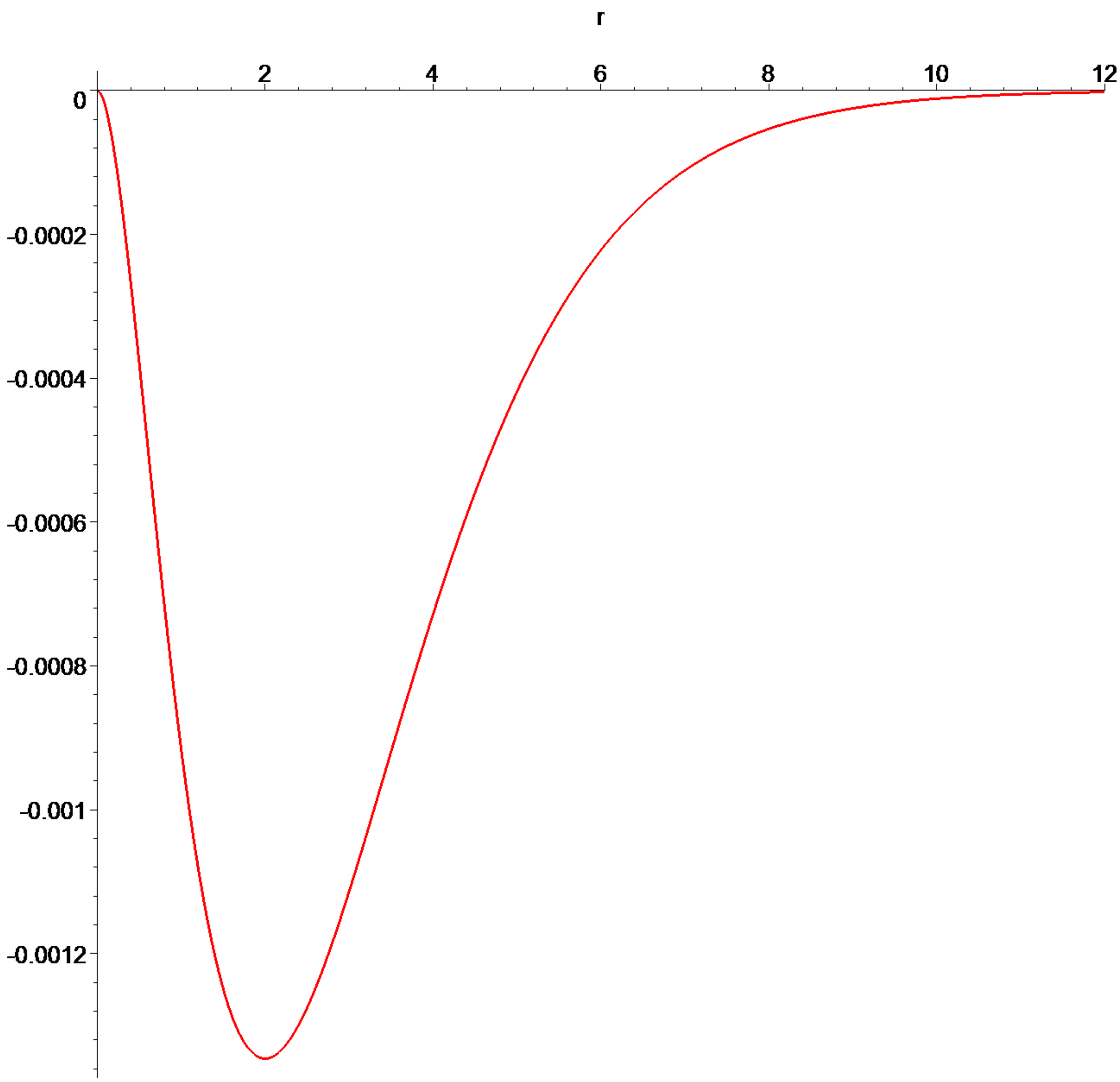
For |2,1,3/2,3/2>,

```
> cc4 :=
  -e*c*alpha*Z^6*r^2*exp(-Z*r/a[0])*sin(theta)^3/(128*Pi*a[0]^5);
```

$$cc4 := -\frac{1}{128}\,\frac{e\,c\,\alpha\,Z^6\,r^2\,\mathbf{e}^{\left(-\frac{Z\,r}{a_0}\right)}\,\sin(\theta)^3}{\pi\,a_0^{\;5}}$$

```
> plot(eval(cc4, [op(cond),theta=Pi/2]), r=0..12, colour=red,
  titlefont=[TIMES,BOLD,14],
          title="profile of circulating current density for
  |2,1,3/2,3/2>", thickness=3);
```

profile of circulating current density for |2,1,3/2,3/2>

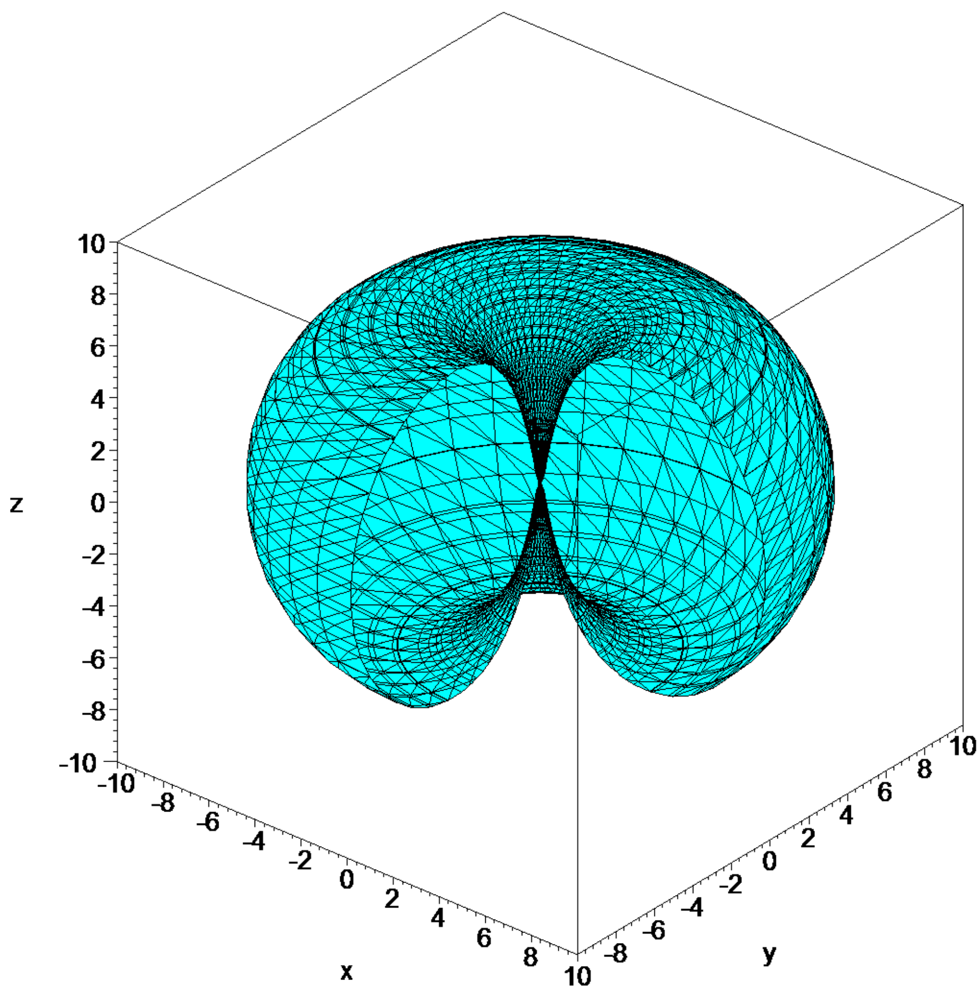



```
>
```

the current density circulates in only one direction.

```
> plots[implicitplot3d](eval(cc4, cond)=-0.0000133, r=0..12,
  theta=0..Pi, phi=0..3/2*Pi,
     colour=cyan, orientation=[-50,60],coords = scispherical,
  grid=[30,30,30], axes=box,
     scaling=constrained, title="circulating current density
  |2,1,3/2,3/2>",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
  view=[-10..10,-10..10,-10..10]);
```

circulating current density |2,1,3/2,3/2>




```
>
```

For |2,1,3/2,1/2>,

```
> cc5 :=
  -e*c*alpha*Z^6*r^2*sin(theta)*(6*cos(theta)^2-1)*exp(-Z*r/a[0])
```

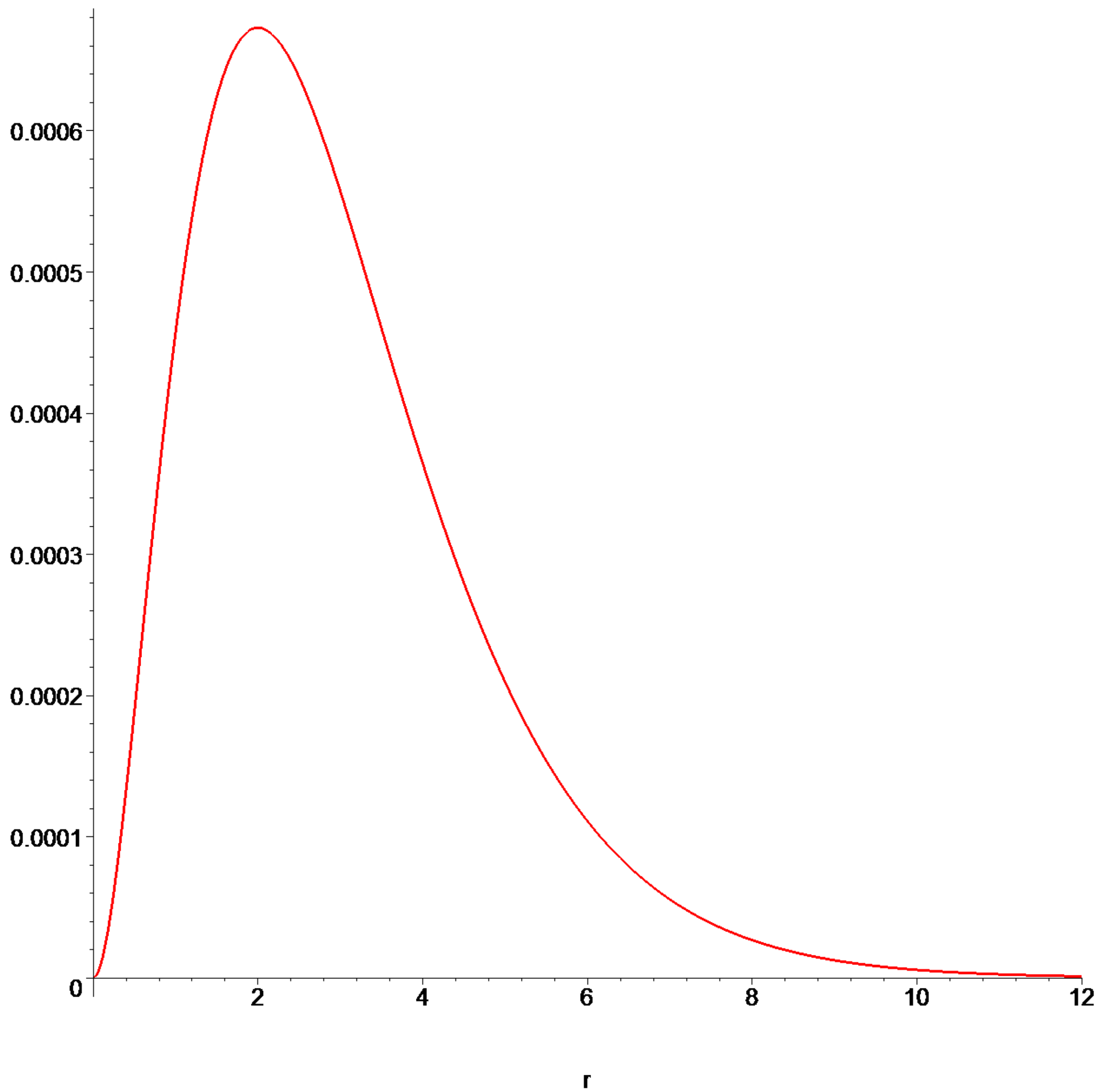
```
/(256*Pi*a[0]^5);
```

$$cc5 := -\frac{1}{256}\,\frac{e\,c\,\alpha\,Z^6\,r^2\,\sin(\theta)\,(6\cos(\theta)^2-1)\,\mathbf{e}^{\left(-\frac{Z\,r}{a_0}\right)}}{\pi\,a_0^{\;5}}$$

the circulating current density has this profile.

```
> plot(eval(cc5, [op(cond),theta=Pi/2]), r=0..12, colour=red,
  titlefont=[TIMES,BOLD,14],
          title="profile of circulating current density for
  |2,1,1/2,1/2>", thickness=3);
```

profile of circulating current density for |2,1,1/2,1/2>

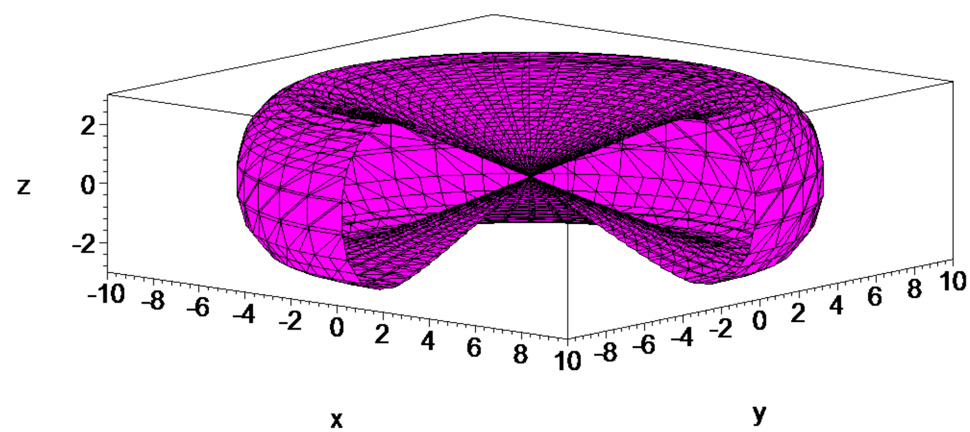



```
>
```

In this case the current density circulates only near plane $z = 0$.

```
> plots[implicitplot3d](eval(cc5, cond)=0.0000066, r=0..15,
  theta=0..Pi, phi=0..3/2*Pi,
     colour=magenta, orientation=[-50,80],coords = scispherical,
  grid=[30,30,30], axes=box,
     scaling=constrained, title="circulating current density
  |2,1,3/2,1/2>",
     labels=["x","y","z"], titlefont=[TIMES,BOLD,14],
  view=[-10..10,-10..10,-3..3]);
```

circulating current density |2,1,3/2,1/2>



>

The changes of colour within two plots above indicate the reversal of the direction of flow of the circulating current in a direction perpendicular to the polar axis in those two cases, |2,0,1/2,1/2> and |2,1,1/2,1/2>.

The fact that Dirac's velocity matrices, of which the component matrices are denoted $\alpha1_x$, $\alpha1_y$, $\alpha1_z$ above, all to be multiplied by c, fail to commute, as we test above, implies that the velocity of an electron in the hydrogen atom fails to be well defined; only one projection of the velocity can be defined, which implies a possibly complicated motion as a sum of a translation and an oscillation with a great frequency that is unobservable because of indeterminacy.

We state above that the expressions for the components of the amplitude functions given by Powell are approximate. For particular case |1,0,1/2,1/2>, we here indicate more accurate expressions.for the three non-zero components.

$$\psi_{1,0,\frac{1}{2},\frac{1}{2}} = N \begin{bmatrix} (1+\gamma)\, r^{(\gamma-1)}\, \mathbf{e}^{\left(-\frac{2\pi Z \alpha m_e c r}{h}\right)} \\ 0 \\ i Z \alpha z\, r^{(\gamma-2)}\, \mathbf{e}^{\left(-\frac{2\pi Z \alpha m_e c r}{h}\right)} \\ i Z \alpha (x + i y)\, r^{(\gamma-2)}\, \mathbf{e}^{\left(-\frac{2\pi Z \alpha m_e c r}{h}\right)} \end{bmatrix}$$

in which appear normalizing factor $N = \sqrt{\dfrac{Z^3}{\pi a_0^{\,3}\left(1+\dfrac{Z^2\alpha^2}{4}\right)}}$ and $\gamma = \sqrt{1 - Z^2\alpha^2}$ in this case. As γ is slightly less than unity, first component ψ_1 is similar to an exponentially decreasing function of r except that at small r this quantity diverges, but this behaviour occurs at a value of r smaller than the radius of a proton. An expansion of these vectorial components in Z or α yields an approximate amplitude function of the form specified above, as we here test with the coefficients of the exponential terms.

```
> restart:
> f := (1+gam)*r^(gam-1);
```

$$f := (1 + gam)\, r^{(gam-1)}$$

```
> taylor(eval(f, gam=sqrt(1-Z^2*alpha^2)), Z=0, 5);
```

$$2 + \left(-\alpha^2 \ln(r) - \frac{\alpha^2}{2}\right) Z^2 + \left(\frac{1}{4}\alpha^4 \ln(r)^2 - \frac{\alpha^4}{8}\right) Z^4 + O(Z^6)$$

```
> f := i*Z*alpha*z*r^(gam-2);
```

$$f := i\, Z\, \alpha\, z\, r^{(gam-2)}$$

```
> taylor(eval(f, [gam=sqrt(1-Z^2*alpha^2), z=r*cos(theta)]), Z=0,
  5);
```

$$i\,\alpha \cos(\theta)\, Z - \frac{1}{2} i\, \alpha^3 \cos(\theta) \ln(r)\, Z^3 + O(Z^5)$$

```
> f := I*Z*alpha*(x+I*y)*r^(gam-2);
```

$$f := Z\, \alpha\, (x + y\, I)\, r^{(gam-2)}\, I$$

```
> map(simplify, taylor(eval(f, [gam=sqrt(1-Z^2*alpha^2),
  x=r*sin(theta)*sin(phi), y=sin(theta)*cos(phi)]), Z=0, 5));
```

$$\frac{\alpha \sin(\theta)\,(\cos(\phi)\,I+\sin(\phi)\,r)\,I}{r}Z+\frac{\frac{-1}{2}I\,\alpha^3\ln(r)\sin(\theta)\,(\cos(\phi)\,I+\sin(\phi)\,r)}{r}Z^3+\mathrm{O}(Z^5)$$

The Dirac equation is not exact: its predictions differ slightly from experimental results as mentioned earlier; more accurate results take account of radiative corrections arising from quantum electrodynamics (Lamb shift) and hyperfine structure attributed to the intrinsic angular momentum of the proton as atomic nucleus of ^{1}H. The electronic mass, m_e, is carried through the equations above, but a further inaccuracy thereby arises; in the treatment of the Schroedinger equation for the hydrogen atom in spherical polar coordinates, we proceeded in terms of a reduced mass, μ, of the system of atomic nucleus and electron, whereas here the corresponding reduced mass should take into account the relativistic variation of mass of the electron with velocity,

$m_e=\frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$ in which m_0 is the rest mass of the electron.

The Dirac equation for the hydrogen atom might be solvable in other systems of coordinates, beyond the spherical polar coordinates in which we present eigenfunctions above, which would imply that the shapes of the surfaces of the components of the eigenfunctions and of the large and small parts of their squares have only parochial meaning, but any properties, such as the circulating current or the density of electronic charge, are independent of the choice of coordinate system.

```
>
>
```