Atlas of spherical hermonics

Notes on Quantum Mechanics

http://quantum.bu.edu/notes/QuantumMechanics/AtlasOfElectronsInAtoms.pdf
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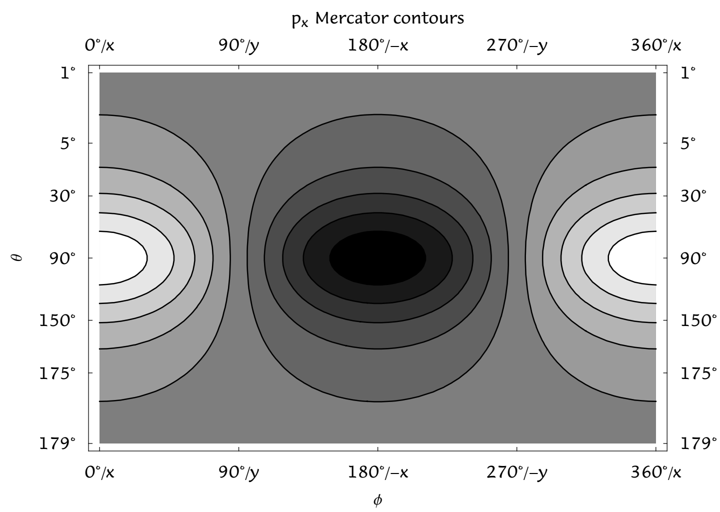
...[quote]...

Here are some ways to visualize real spherical harmonics, the angular parts one electron atom wavefunctions, using p_x as example.

■ Mercator contours

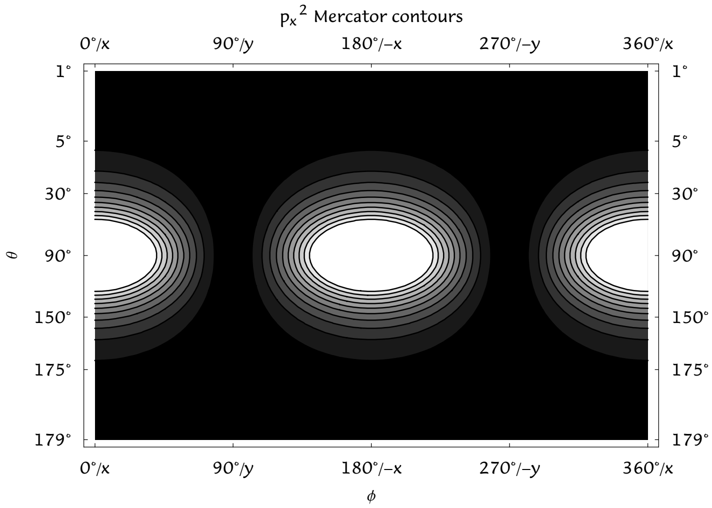
The Mercator projection, commonly used to display maps of Earth, expresses ϕ (longitude) and θ (latitude) on a rectangular grid such that traversing a straight line between two points corresponds to a constant compass bearing. To achieve this effect, distances between points of constant latitude increase moving away from the equator ($\theta = 90°$), and this is why Mercator projections of maps of Earth exaggerate the polar regions (θ near 0° and 180°). Here is are the contours of constant value of the p_x angular function on the Mercator grid.



Mercator contours of the p_x spherical harmonic.

The angle ϕ corresponds to the longitude, with Greenwich ($\phi = 0°$) meridian corresponding to the $+x$ direction. The angle θ corresponds to latitude, with the equator corresponding to $\theta = 90°$. Note that the Mercator projection expands the latitude scale near the poles, $\theta = 0°$, 180°. The light areas correspond to positive values of the angular function and the dark area correspond to negative values.

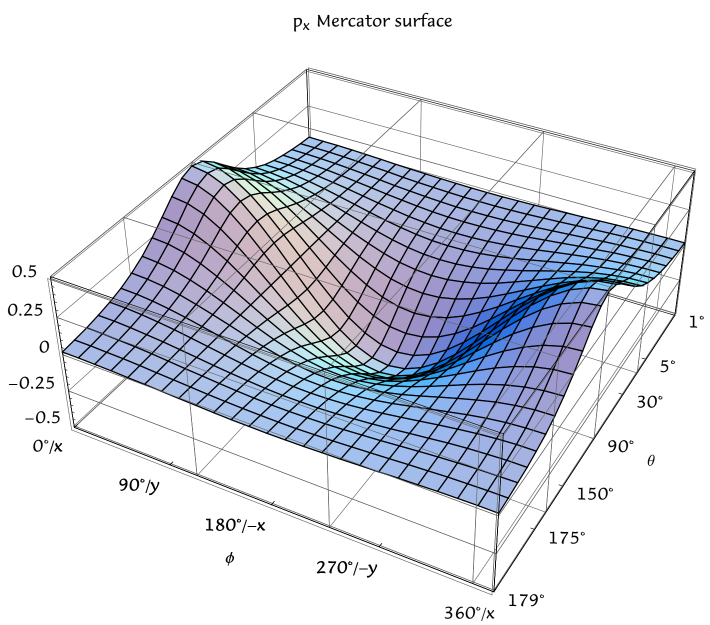
Here are the contours of constant value of the square of the p_x angular function on the Mercator grid.



Mercator contours of the $p_x{}^2$ spherical harmonic angular probability density.

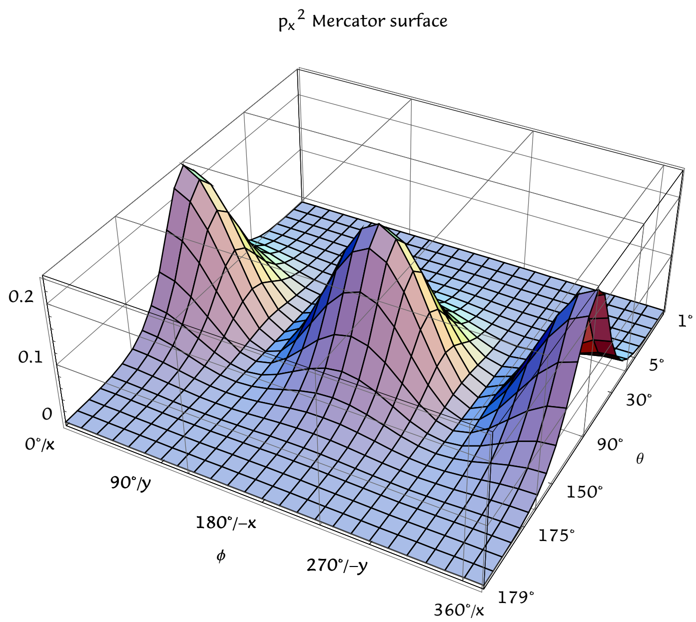
■ Mercator surface

An alternative representation of the Mercator contours is a the Mercator surface.



Mercator surface of the p_x spherical harmonic.

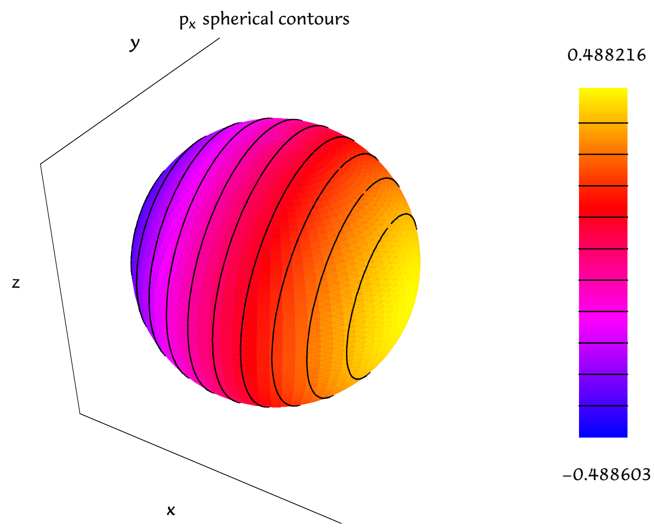
The height or depth of the surface at each point θ, ϕ is the value of the angular function at that point. Here is the surface corresponding to the square of the p_x angular function on the Mercator grid.



Mercator surface of the $p_x{}^2$ spherical harmonic angular probability density.

■ Spherical contours

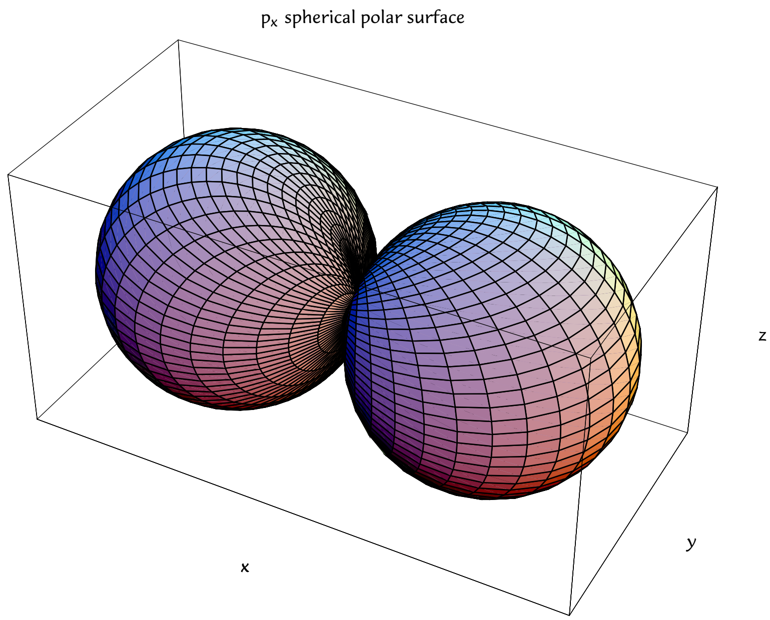
Mercator (or other two dimensional) grids are used to represent the spherical surfaces in two dimensions. Instead, we can maps contours of constant value onto a sphere. Here are the color coded contours of constant value of the p_x angular function.



Contours of the p_x spherical harmonic mapped onto a sphere. The values of the function are indicated by the scale bar on the right.

■ Spherical polar surface

In textbooks the most common representation of angular wavefunctions is known as a spherical polar surface. A spherical polar surface is the surface whose distance from the origin along a particular direction θ, ϕ is the magnitude (that is, the value without sign) of the angular wavefunction along that direction. If the value of the angular wavefunction is positive, a + sign is placed near that part of the surface, and if the value of the angular wavefunction is negative, a – sign is placed near that part of the surface. Here is the p_x spherical polar surface.



Spherical polar surface of the p_x spherical harmonic.

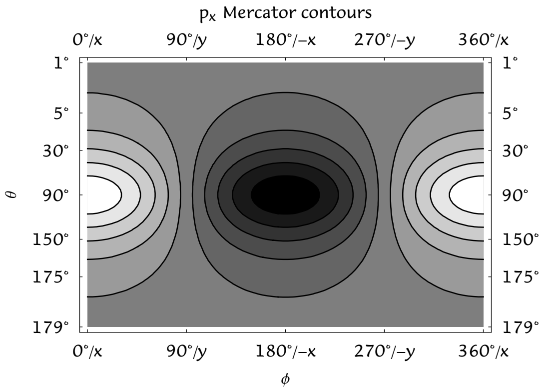
Caution: Spherical polar surfaces of angular wavefunctions are misleading!

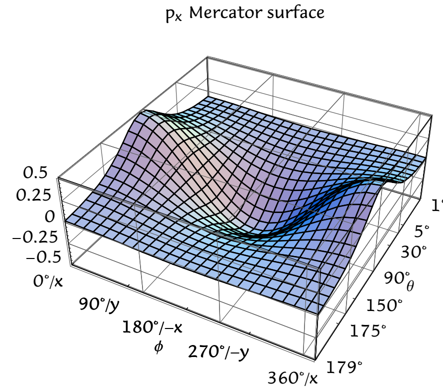
Here is what leads to confusion. The coordinates x, y and z on the spherical polar plot serve *only* to fix the coordinate system used to define the angles θ and ϕ in the other two plots. In particular, these x , y and z coordinates are *not* the coordinates of the use to define the location of the electron in space. It is absolutely crucial that you understand this. The reason is that in the spherical polar plot the distance from the origin along a particular direction is *not* the distance of the electron from the nucleus along that direction; rather this distance is the numerical value of the angular wavefunction along the particular direction.

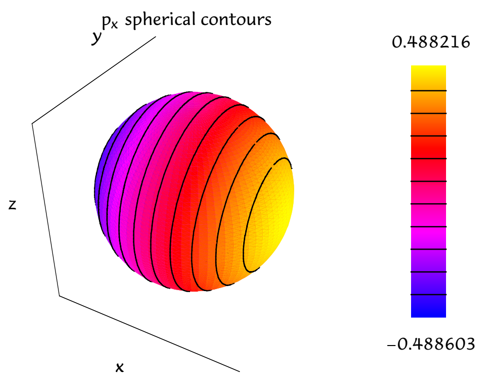
■ Atlas of angular function

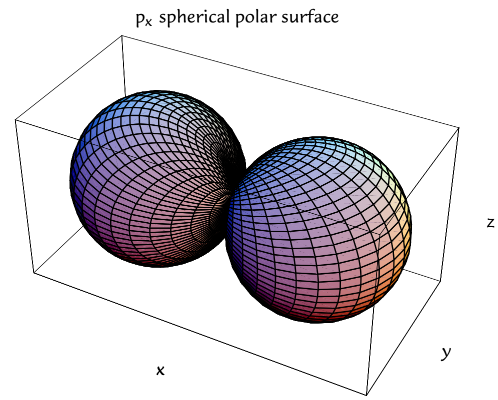
In the following pages collect together the various representations of the angular functions and their squares for the p and d angular functions.

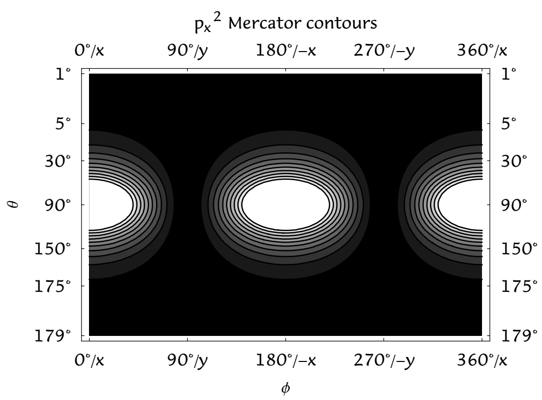
p_x

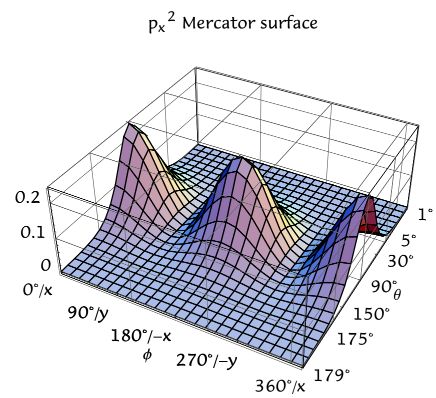

p_x Mercator contours
0°/x 90°/y 180°/−x 270°/−y 360°/x
1° 5° 30° 90° 150° 175° 179°
θ
ϕ


p_x Mercator surface
0.5 0.25 0 −0.25 −0.5
0°/x 90°/y 180°/−x 270°/−y 360°/x
ϕ
1° 5° 30° 90° 150° 175° 179°
θ

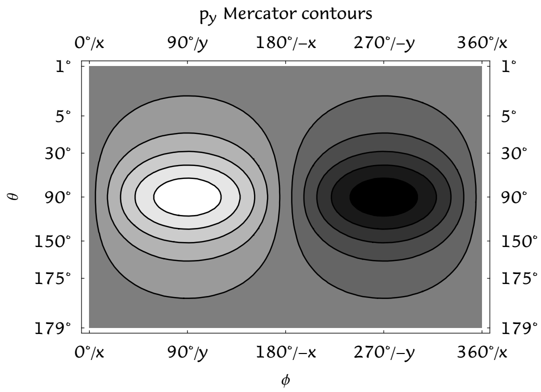

p_x spherical contours
y
z
x
0.488216
−0.488603

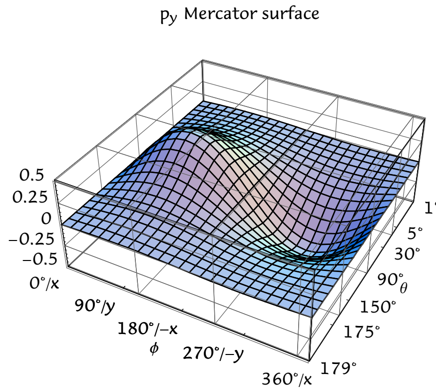

p_x spherical polar surface
z
x
y

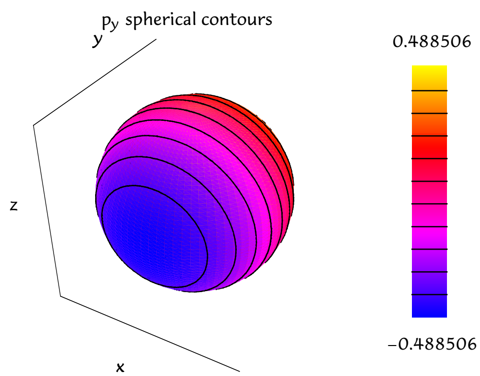

p_x^2 Mercator contours
0°/x 90°/y 180°/−x 270°/−y 360°/x
1° 5° 30° 90° 150° 175° 179°
θ
ϕ

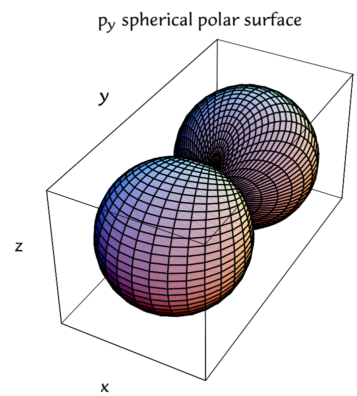

p_x^2 Mercator surface
0.2 0.1 0
0°/x 90°/y 180°/−x 270°/−y 360°/x
ϕ
1° 5° 30° 90° 150° 175° 179°
θ

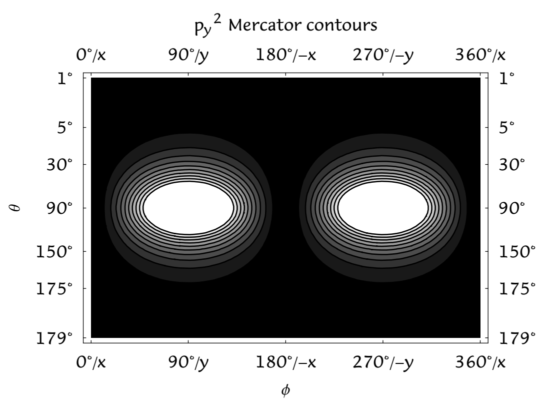
p_y

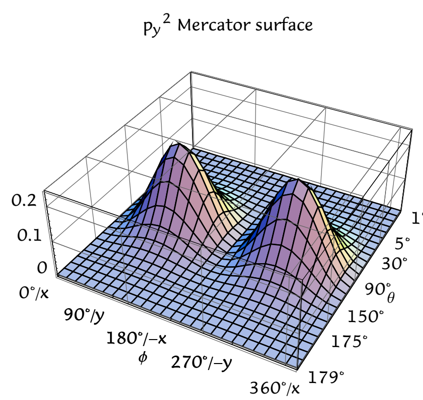

p_y Mercator contours
0°/x
90°/y
180°/−x
270°/−y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ


p_y Mercator surface
0.5
0.25
0
−0.25
−0.5
0°/x
90°/y
180°/−x
ϕ
270°/−y
360°/x
1°
5°
30°
90°
θ
150°
175°
179°

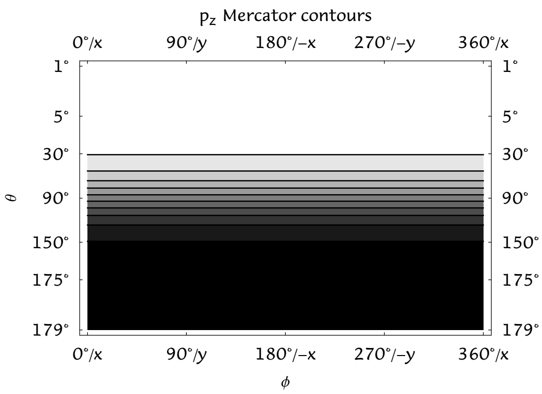

p_y spherical contours
y
z
x
0.488506
−0.488506

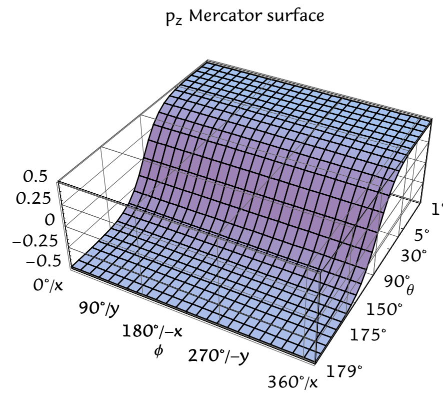

p_y spherical polar surface
y
z
x

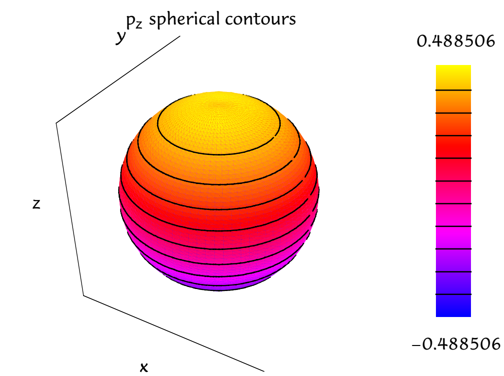

p_y^2 Mercator contours
0°/x
90°/y
180°/−x
270°/−y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ

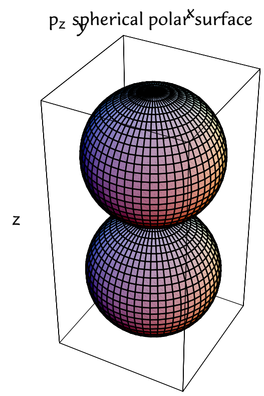

p_y^2 Mercator surface
0.2
0.1
0
0°/x
90°/y
180°/−x
ϕ
270°/−y
360°/x
1°
5°
30°
90°
θ
150°
175°
179°

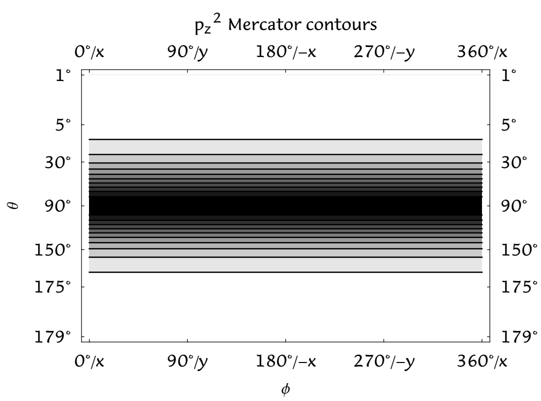
p_z


pz Mercator contours
0°/x
90°/y
180°/–x
270°/–y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ


pz Mercator surface
0.5
0.25
0
–0.25
–0.5
0°/x
90°/y
180°/–x
270°/–y
360°/x
ϕ
1°
5°
30°
90°
θ
150°
175°
179°


pz spherical contours
y
z
x
0.488506
–0.488506


pz spherical polar surface
y
x
z


pz2 Mercator contours
0°/x
90°/y
180°/–x
270°/–y
360°/x
1°
5°
30°
90°
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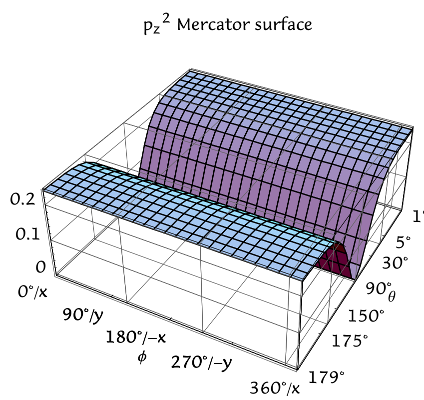
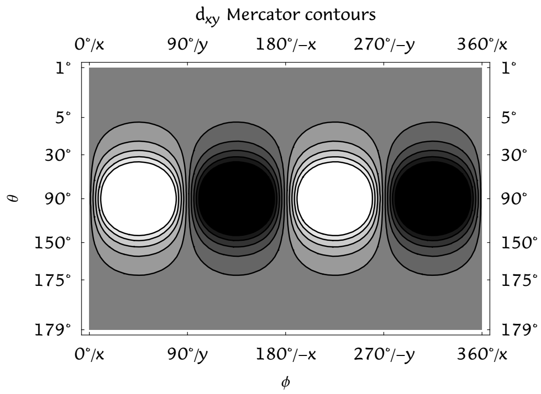
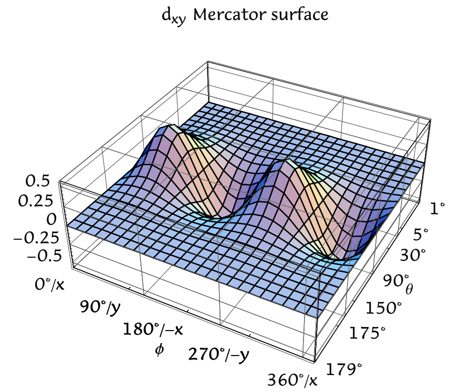
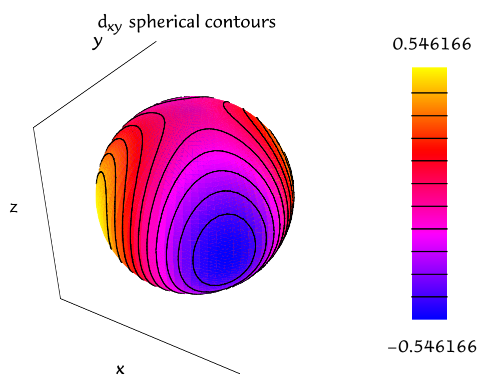
175°
179°
θ
ϕ

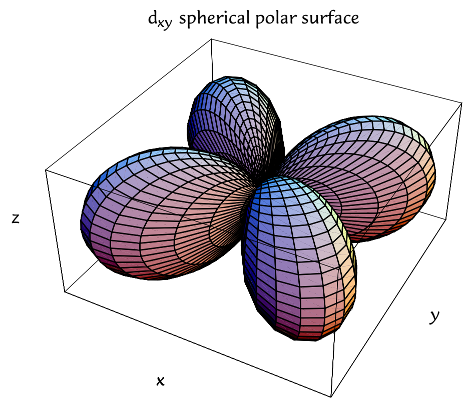

pz2 Mercator surface
0.2
0.1
0
0°/x
90°/y
180°/–x
270°/–y
360°/x
ϕ
1°
5°
30°
90°
θ
150°
175°
179°

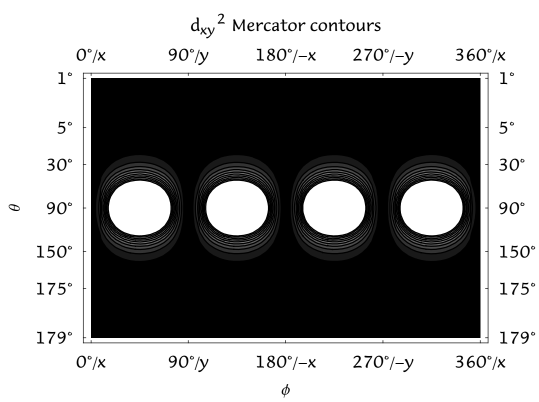
d_{xy}

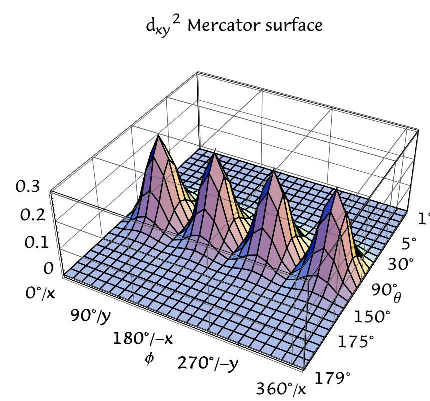

dxy Mercator contours
0°/x 90°/y 180°/–x 270°/–y 360°/x
1° 5° 30° 90° 150° 175° 179°
θ
ϕ


dxy Mercator surface
0.5 0.25 0 –0.25 –0.5
0°/x 90°/y 180°/–x 270°/–y 360°/x
ϕ
1° 5° 30° 90° 150° 175° 179°
θ

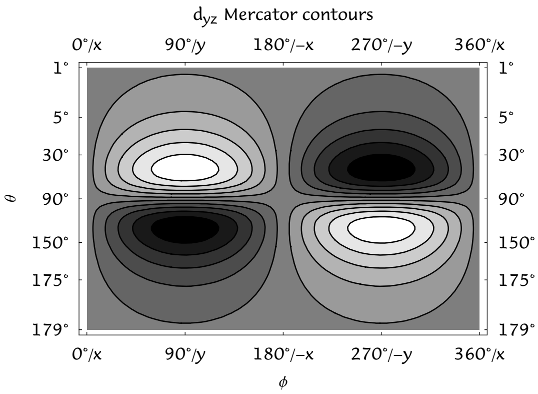

dxy spherical contours
y
z
x
0.546166
–0.546166

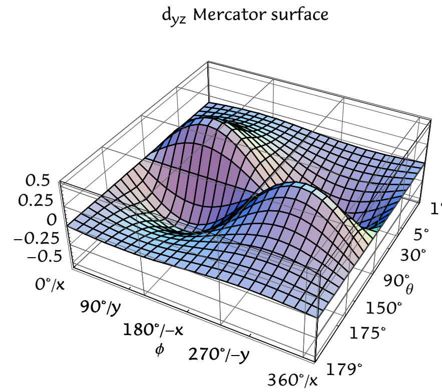

dxy spherical polar surface
z
y
x

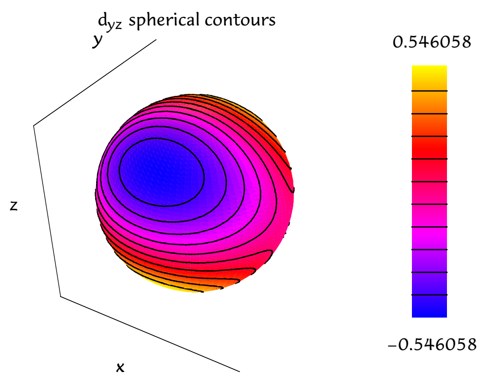

dxy² Mercator contours
0°/x 90°/y 180°/–x 270°/–y 360°/x
1° 5° 30° 90° 150° 175° 179°
θ
ϕ


dxy² Mercator surface
0.3 0.2 0.1 0
0°/x 90°/y 180°/–x 270°/–y 360°/x
ϕ
1° 5° 30° 90° 150° 175° 179°
θ

d_{yz}


dyz Mercator contours
0°/x
90°/y
180°/−x
270°/−y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ


dyz Mercator surface
0.5
0.25
0
−0.25
−0.5
0°/x
90°/y
180°/−x
270°/−y
360°/x
ϕ
1°
5°
30°
90°
150°
175°
179°
θ


dyz spherical contours
y
z
x
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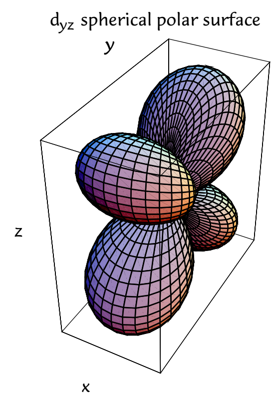
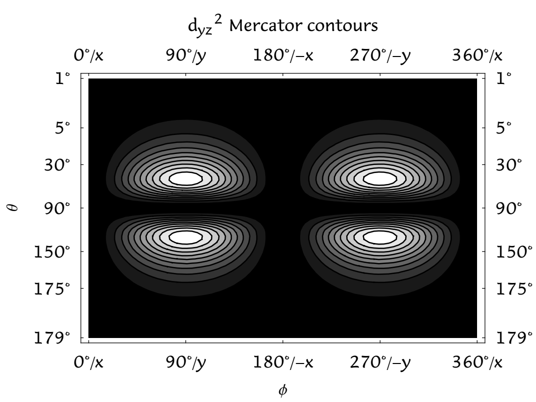
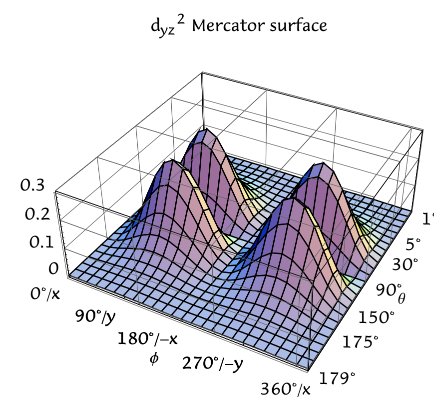
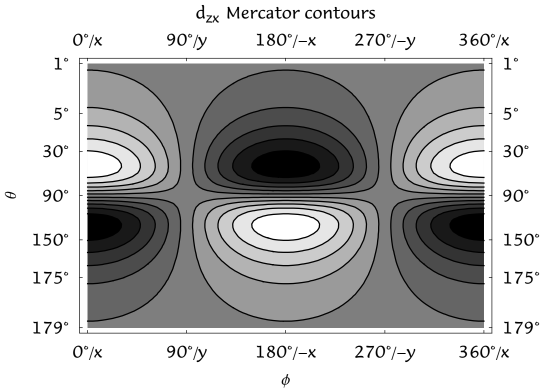
−0.546058


dyz spherical polar surface
y
z
x


dyz2 Mercator contours
0°/x
90°/y
180°/−x
270°/−y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ


dyz2 Mercator surface
0.3
0.2
0.1
0
0°/x
90°/y
180°/−x
270°/−y
360°/x
ϕ
1°
5°
30°
90°
150°
175°
179°
θ

d_{zx}


dzx Mercator contours
0°/x
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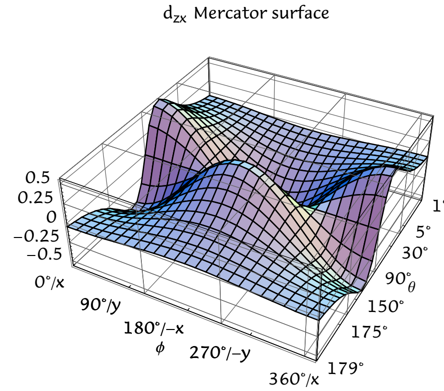
270°/−y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ


dzx Mercator surface
0.5
0.25
0
−0.25
−0.5
0°/x
90°/y
180°/−x
270°/−y
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ϕ
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5°
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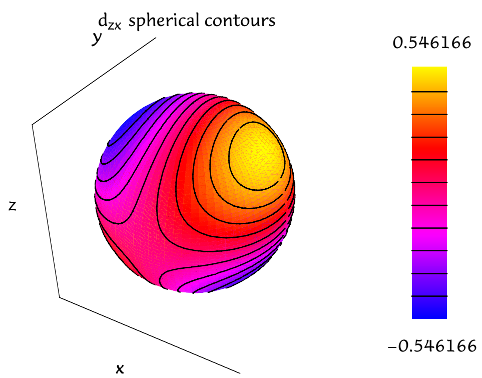
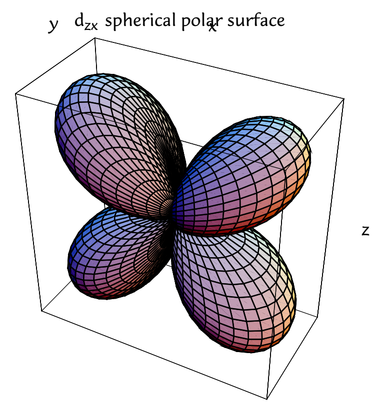
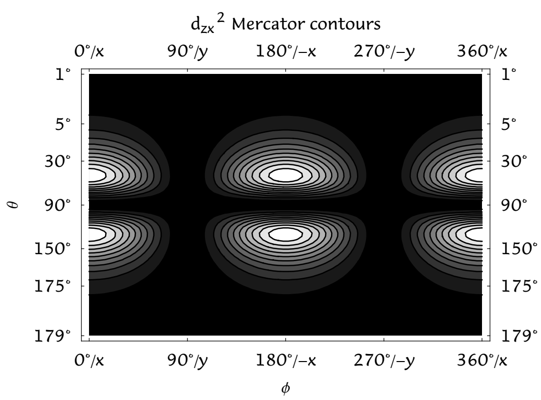
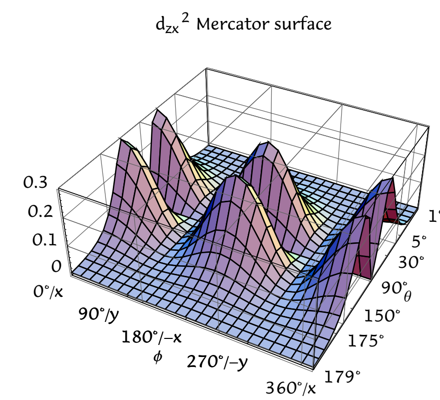
90°
150°
175°
179°
θ

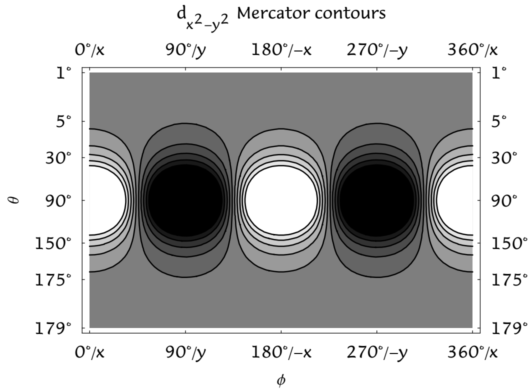

dzx spherical contours
y
z
x
0.546166
−0.546166

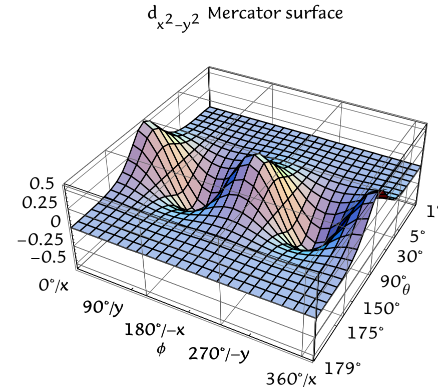

y
dzx spherical polar surface
x
z

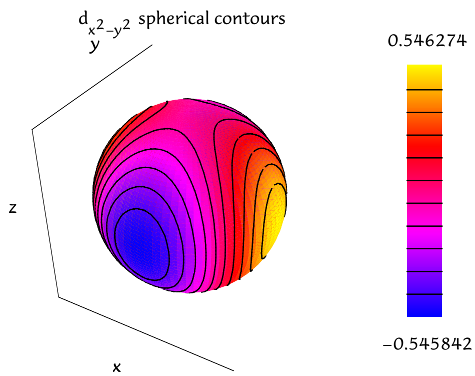

dzx 2 Mercator contours
0°/x
90°/y
180°/−x
270°/−y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ

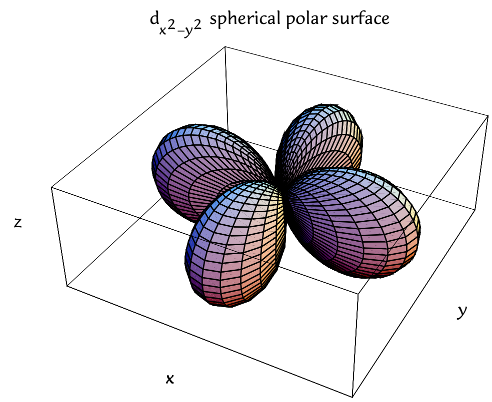

dzx 2 Mercator surface
0.3
0.2
0.1
0
0°/x
90°/y
180°/−x
270°/−y
360°/x
ϕ
1°
5°
30°
90°
150°
175°
179°
θ

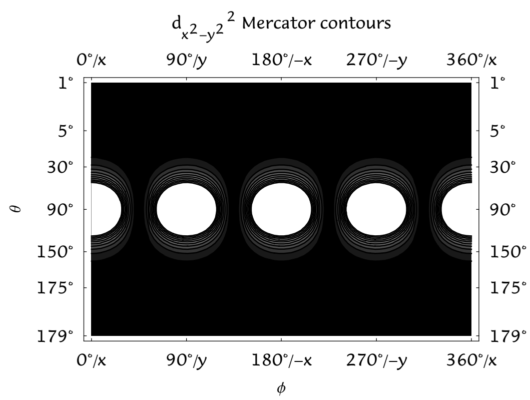
$d_{x^2-y^2}$

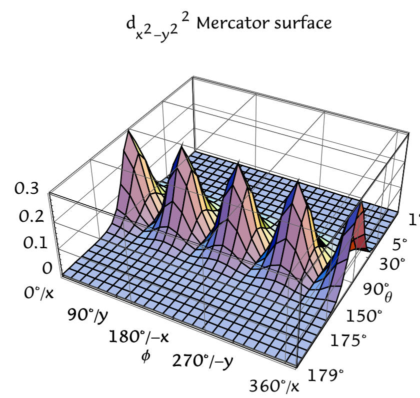

d x2−y2 Mercator contours
0°/x 90°/y 180°/−x 270°/−y 360°/x
1° 5° 30° 90° 150° 175° 179°
θ
ϕ


d x2−y2 Mercator surface
0.5 0.25 0 −0.25 −0.5
0°/x 90°/y 180°/−x 270°/−y 360°/x
ϕ
1° 5° 30° 90° 150° 175° 179°
θ

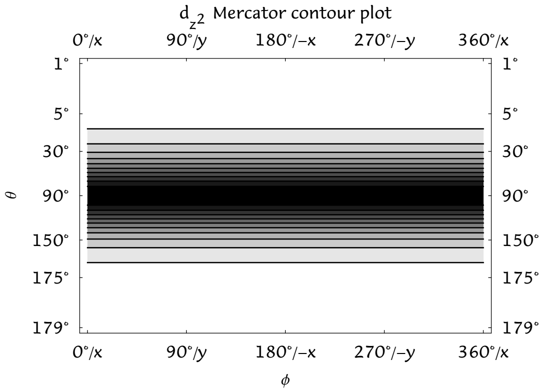

d x2−y2 spherical contours
y
z
x
0.546274
−0.545842

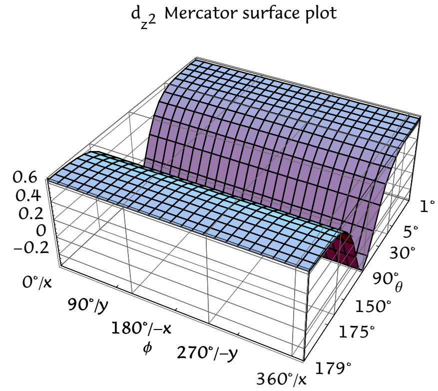

d x2−y2 spherical polar surface
z
y
x

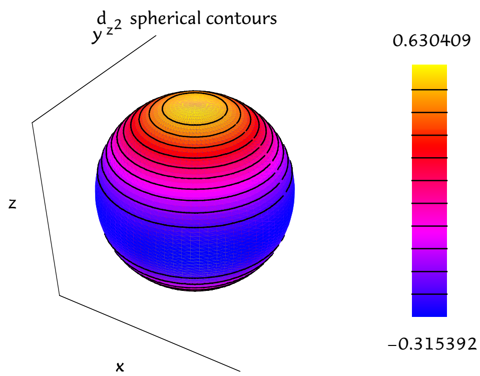

d x2−y2 2 Mercator contours
0°/x 90°/y 180°/−x 270°/−y 360°/x
1° 5° 30° 90° 150° 175° 179°
θ
ϕ

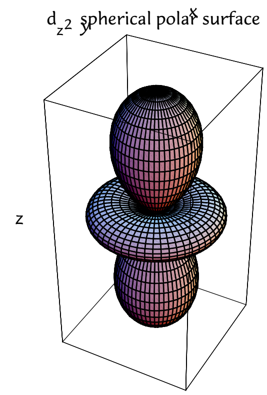

d x2−y2 2 Mercator surface
0.3 0.2 0.1 0
0°/x 90°/y 180°/−x 270°/−y 360°/x
ϕ
1° 5° 30° 90° 150° 175° 179°
θ

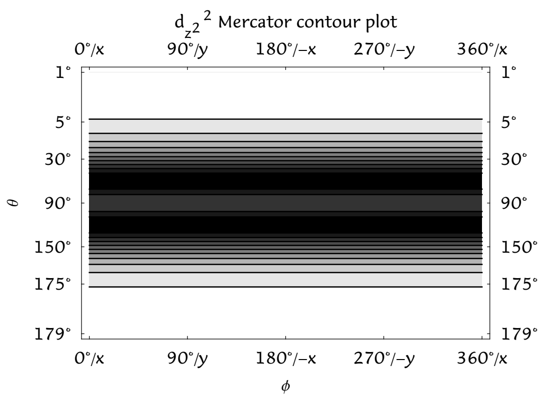
d_{z^2}

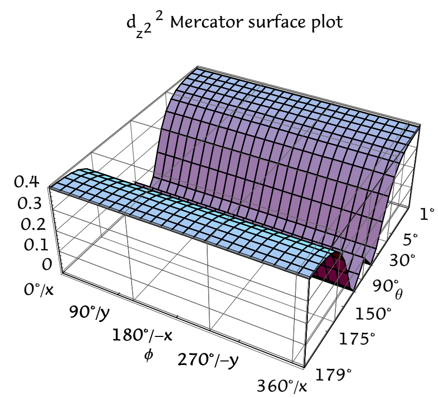

d z2 Mercator contour plot
0°/x
90°/y
180°/−x
270°/−y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ


d z2 Mercator surface plot
0.6
0.4
0.2
0
−0.2
0°/x
90°/y
180°/−x
270°/−y
360°/x
ϕ
1°
5°
30°
90°
150°
175°
179°
θ


d z2 spherical contours
0.630409
−0.315392
y
z
x


d z2 spherical polar surface
y
x
z


d z2 2 Mercator contour plot
0°/x
90°/y
180°/−x
270°/−y
360°/x
1°
5°
30°
90°
150°
175°
179°
θ
ϕ


d z2 2 Mercator surface plot
0.4
0.3
0.2
0.1
0
0°/x
90°/y
180°/−x
270°/−y
360°/x
ϕ
1°
5°
30°
90°
150°
175°
179°
θ