

Orbital angular momentum and the spherical harmonics

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1 Orbital angular momentum

We compare our result on representations of rotations with our previous experience of angular momentum, defined for a point particle as

$$\mathbf{L} = \mathbf{x} \times \mathbf{p}$$

or, for a quantum system as the operator relationship

$$\hat{\mathbf{L}} = \hat{\mathbf{x}} \times \hat{\mathbf{p}}$$

Notice that since

$$\hat{L}_i = \varepsilon_{ijk} \hat{x}_j \hat{p}_k$$

there is no ordering ambiguity: \hat{x}_j and \hat{p}_k commute as long as $j \neq k$, and the cross product insures this. Computing commutators, we have

$$\begin{aligned} [\hat{L}_i, \hat{L}_m] &= [\varepsilon_{ijk} \hat{x}_j \hat{p}_k, \varepsilon_{mns} \hat{x}_n \hat{p}_s] \\ &= \varepsilon_{ijk} \varepsilon_{mns} [\hat{x}_j \hat{p}_k, \hat{x}_n \hat{p}_s] \\ &= \varepsilon_{ijk} \varepsilon_{mns} (\hat{x}_j [\hat{p}_k, \hat{x}_n \hat{p}_s] + [\hat{x}_j, \hat{x}_n \hat{p}_s] \hat{p}_k) \\ &= \varepsilon_{ijk} \varepsilon_{mns} (\hat{x}_j [\hat{p}_k, \hat{x}_n] \hat{p}_s + \hat{x}_n [\hat{x}_j, \hat{p}_s] \hat{p}_k) \\ &= \varepsilon_{ijk} \varepsilon_{mns} (-i\hbar \delta_{kn} \hat{x}_j \hat{p}_s + i\hbar \delta_{js} \hat{x}_n \hat{p}_k) \\ &= i\hbar (-\varepsilon_{ijk} \varepsilon_{mks} \hat{x}_j \hat{p}_s + \varepsilon_{ijk} \varepsilon_{mnj} \hat{x}_n \hat{p}_k) \\ &= i\hbar ((\delta_{im} \delta_{js} - \delta_{is} \delta_{jm}) \hat{x}_j \hat{p}_s - (\delta_{im} \delta_{kn} - \delta_{in} \delta_{km}) \hat{x}_n \hat{p}_k) \\ &= i\hbar (\delta_{im} \hat{x}_j \hat{p}_j - \hat{x}_m \hat{p}_i - \delta_{im} \hat{x}_k \hat{p}_k + \hat{x}_i \hat{p}_m) \\ &= i\hbar (-\hat{x}_m \hat{p}_i + \hat{x}_i \hat{p}_m) \end{aligned}$$

Therefore, with

$$\begin{aligned} \varepsilon_{imn} \hat{L}_i &= \varepsilon_{imn} \varepsilon_{ijk} \hat{x}_j \hat{p}_k \\ &= (\delta_{mj} \delta_{nk} - \delta_{mk} \delta_{nj}) \hat{x}_j \hat{p}_k \\ &= \hat{x}_m \hat{p}_n - \hat{x}_n \hat{p}_m \end{aligned}$$

this becomes

$$[\hat{L}_i, \hat{L}_m] = i\hbar \varepsilon_{imn} \hat{L}_n$$

and we see that \hat{L}_m satisfies the angular momentum commutation relations and must therefore admit $|l, m\rangle$ representations satisfying

$$\begin{aligned} \hat{L}_z |l, m\rangle &= m\hbar |l, m\rangle \\ \hat{\mathbf{L}}^2 |l, m\rangle &= l(l+1)\hbar^2 |l, m\rangle \end{aligned}$$

along with raising and lowering operators, \hat{L}_\pm . However, in this case we have an explicit coordinate representation for the operators. For the z -component,

$$\begin{aligned}\langle \mathbf{x} | \hat{L}_3 | \alpha \rangle &= \langle \mathbf{x} | (\hat{x}_1 \hat{p}_2 - \hat{x}_2 \hat{p}_1) | \alpha \rangle \\ &= -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \langle \mathbf{x} | \alpha \rangle\end{aligned}$$

Similarly, the x - and y -components are

$$\begin{aligned}\langle \mathbf{x} | \hat{L}_1 | \alpha \rangle &= -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \langle \mathbf{x} | \alpha \rangle \\ \langle \mathbf{x} | \hat{L}_2 | \alpha \rangle &= -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \langle \mathbf{x} | \alpha \rangle\end{aligned}$$

so we may construct the raising and lowering operators,

$$\begin{aligned}\langle \mathbf{x} | \hat{L}_\pm | \alpha \rangle &= -i\hbar \left[\left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \pm i \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \right] \langle \mathbf{x} | \alpha \rangle \\ &= -i\hbar \left[\pm iz \frac{\partial}{\partial x} - z \frac{\partial}{\partial y} \mp i(x \pm iy) \frac{\partial}{\partial z} \right] \langle \mathbf{x} | \alpha \rangle\end{aligned}$$

This exposes an essential asymmetry between spinors and vectors. We have seen that 3-vectors may be represented a matrices in a complex, 2-dim spinor representation, there does not exist a similar representation of spinors using 3-dim coordinates. Thus, since orbital angular momentum operators may be written in a coordinate representation, we will see that they only admit integer j representations, so the states $|l, m\rangle$ only exist for integer l . To see this in detail, we need to change from Cartesian to spherical coordinates.

2 Changing to spherical coordinates

Here we rewrite \hat{L}_z, \hat{L}_\pm and $\hat{\mathbf{L}}^2$ in spherical coordinates. The coordinate transformation and its inverse are given by

$$\begin{aligned}r &= \sqrt{x^2 + y^2 + z^2} \\ \theta &= \tan^{-1} \left(\frac{x^2 + y^2}{r^2} \right) \\ \varphi &= \tan^{-1} \left(\frac{y}{x} \right)\end{aligned}$$

and

$$\begin{aligned}x &= r \sin \theta \cos \varphi \\ y &= r \sin \theta \sin \varphi \\ z &= r \cos \theta\end{aligned}$$

We also need the derivative operators, $\frac{\partial}{\partial x^i}$. Using the chain rule, we have

$$\begin{aligned}\frac{\partial}{\partial x} &= \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x} \frac{\partial}{\partial \varphi} \\ \frac{\partial}{\partial y} &= \frac{\partial r}{\partial y} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y} \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial y} \frac{\partial}{\partial \varphi} \\ \frac{\partial}{\partial z} &= \frac{\partial r}{\partial z} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z} \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial z} \frac{\partial}{\partial \varphi}\end{aligned}$$

Computing the partial derivatives, we start with the differential of r ,

$$dr = \frac{x}{r} dx + \frac{y}{r} dy + \frac{z}{r} dz$$

and read off

$$\begin{aligned} \frac{\partial r}{\partial x} &= \frac{x}{r} \\ \frac{\partial r}{\partial y} &= \frac{y}{r} \\ \frac{\partial r}{\partial z} &= \frac{z}{r} \end{aligned}$$

Next, for θ , we take the differential of $\tan \theta$,

$$\begin{aligned} \tan \theta &= \frac{\sqrt{x^2 + y^2}}{z} \\ \frac{1}{\cos^2 \theta} d\theta &= \frac{1}{\sqrt{x^2 + y^2}} \frac{x}{z} dx + \frac{1}{\sqrt{x^2 + y^2}} \frac{y}{z} dy - \frac{\sqrt{x^2 + y^2}}{z^2} dz \end{aligned}$$

Then, since

$$\cos^2 \theta = \frac{z^2}{r^2}$$

we have

$$d\theta = \frac{1}{\sqrt{x^2 + y^2}} \frac{xz}{r^2} dx + \frac{1}{\sqrt{x^2 + y^2}} \frac{yz}{r^2} dy - \frac{\sqrt{x^2 + y^2}}{r^2} dz$$

and read off the partials,

$$\begin{aligned} \frac{\partial \theta}{\partial x} &= \frac{1}{\sqrt{x^2 + y^2}} \frac{xz}{r^2} \\ \frac{\partial \theta}{\partial y} &= \frac{1}{\sqrt{x^2 + y^2}} \frac{yz}{r^2} \\ \frac{\partial \theta}{\partial z} &= -\frac{\sqrt{x^2 + y^2}}{r^2} \end{aligned}$$

Finally, we compute the differential of $\tan \varphi = \frac{y}{x}$, and use $\cos^2 \varphi = \frac{x^2}{x^2 + y^2}$

$$\begin{aligned} \frac{1}{\cos^2 \varphi} d\varphi &= \frac{1}{x} dy - \frac{y}{x^2} dx \\ d\varphi &= \frac{x}{x^2 + y^2} dy - \frac{y}{x^2 + y^2} dx \end{aligned}$$

and once again read off the partials

$$\begin{aligned} \frac{\partial \varphi}{\partial x} &= -\frac{y}{x^2 + y^2} \\ \frac{\partial \varphi}{\partial y} &= \frac{x}{x^2 + y^2} \\ \frac{\partial \varphi}{\partial z} &= 0 \end{aligned}$$

Now, returning to the chain rule expansions, we substitute to find

$$\begin{aligned}
\frac{\partial}{\partial x} &= \frac{x}{r} \frac{\partial}{\partial r} + \frac{1}{\sqrt{x^2 + y^2}} \frac{xz}{r^2} \frac{\partial}{\partial \theta} - \frac{y}{x^2 + y^2} \frac{\partial}{\partial \varphi} \\
&= \sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{1}{r} \frac{\sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \\
\frac{\partial}{\partial y} &= \frac{y}{r} \frac{\partial}{\partial r} + \frac{1}{\sqrt{x^2 + y^2}} \frac{yz}{r^2} \frac{\partial}{\partial \theta} + \frac{x}{x^2 + y^2} \frac{\partial}{\partial \varphi} \\
&= \sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{1}{r} \frac{\cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \\
\frac{\partial}{\partial z} &= \frac{z}{r} \frac{\partial}{\partial r} - \frac{\sqrt{x^2 + y^2}}{r^2} \frac{\partial}{\partial \theta} \\
&= \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta}
\end{aligned}$$

and we may substitute into the orbital angular momentum operators.

3 Orbital angular momentum operators in spherical coordinates

Carrying out the coordinate substitutions, for \hat{L}_3 we have

$$\begin{aligned}
-i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) &= -i\hbar r \sin \theta \cos \varphi \left(\sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{1}{r} \frac{\cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \\
&\quad + i\hbar r \sin \theta \sin \varphi \left(\sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{1}{r} \frac{\sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \\
&= -i\hbar \frac{\partial}{\partial \varphi}
\end{aligned}$$

For the raising operator, we have

$$\begin{aligned}
\frac{1}{\hbar} \hat{L}_+ &= z \frac{\partial}{\partial x} + iz \frac{\partial}{\partial y} - (x + iy) \frac{\partial}{\partial z} \\
&= r \cos \theta \left(\sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{1}{r} \frac{\sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \\
&\quad + r \cos \theta \left(i \sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{i}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{i}{r} \frac{\cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \\
&\quad - r \sin \theta (\cos \varphi + i \sin \varphi) \left(\cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right) \\
&= (\cos \varphi + i \sin \varphi - e^{i\varphi}) r \cos \theta \sin \theta \frac{\partial}{\partial r} + \cos^2 \theta e^{i\varphi} \frac{\partial}{\partial \theta} + e^{i\varphi} \sin^2 \theta \frac{\partial}{\partial \theta} \\
&\quad + i (\cos \varphi + i \sin \varphi) \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \\
&= e^{i\varphi} \left(\frac{\partial}{\partial \theta} + i \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \right)
\end{aligned}$$

while the lowering operator is

$$\frac{1}{\hbar} \hat{L}_- = -z \frac{\partial}{\partial x} + iz \frac{\partial}{\partial y} + (x - iy) \frac{\partial}{\partial z}$$

$$\begin{aligned}
&= -r \cos \theta \left(\sin \theta \cos \varphi \frac{\partial}{\partial r} + \frac{1}{r} \cos \theta \cos \varphi \frac{\partial}{\partial \theta} - \frac{1}{r} \frac{\sin \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \\
&\quad + r \cos \theta \left(i \sin \theta \sin \varphi \frac{\partial}{\partial r} + \frac{i}{r} \cos \theta \sin \varphi \frac{\partial}{\partial \theta} + \frac{i}{r} \frac{\cos \varphi}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \\
&\quad + r \sin \theta (\cos \varphi - i \sin \varphi) \left(\cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right) \\
&= r e^{-i\varphi} \sin \theta \cos \theta \frac{\partial}{\partial r} - r e^{-i\varphi} \cos \theta \sin \theta \frac{\partial}{\partial r} \\
&\quad - e^{-i\varphi} \cos^2 \theta \frac{\partial}{\partial \theta} - e^{-i\varphi} \sin^2 \theta \frac{\partial}{\partial \theta} + i e^{-i\varphi} \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \\
&= -e^{-i\varphi} \frac{\partial}{\partial \theta} + i e^{-i\varphi} \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi}
\end{aligned}$$

Collecting these,

$$\begin{aligned}
\hat{L}_+ &= \hbar e^{i\varphi} \left(\frac{\partial}{\partial \theta} + i \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \\
\hat{L}_- &= \hbar e^{-i\varphi} \left(-\frac{\partial}{\partial \theta} + i \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \right)
\end{aligned}$$

Finally, since

$$\hat{L}_+ \hat{L}_- = \mathbf{L}^2 - L_3^2 + \hbar L_3$$

we have

$$\begin{aligned}
\mathbf{L}^2 &= \hat{L}_+ \hat{L}_- + L_3^2 - \hbar L_3 \\
&= \hbar e^{i\varphi} \left(\frac{\partial}{\partial \theta} + i \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \left[\hbar e^{-i\varphi} \left(-\frac{\partial}{\partial \theta} + i \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \right] + \left(-i\hbar \frac{\partial}{\partial \varphi} \right)^2 + i\hbar^2 \frac{\partial}{\partial \varphi} \\
&= -\hbar^2 \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \theta} + i\hbar^2 \frac{\cos^2 \theta}{\sin^2 \theta} \frac{\partial}{\partial \varphi} \\
&\quad - \hbar^2 \frac{\partial^2}{\partial \theta^2} - i\hbar^2 \frac{\cos \theta}{\sin \theta} \frac{\partial^2}{\partial \varphi \partial \theta} + i\hbar^2 \left(-1 - \frac{\cos^2 \theta}{\sin^2 \theta} \right) \frac{\partial}{\partial \varphi} \\
&\quad + i\hbar^2 \frac{\cos \theta}{\sin \theta} \frac{\partial^2}{\partial \theta \partial \varphi} - \hbar^2 \frac{\cos^2 \theta}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \\
&\quad - \hbar^2 \frac{\partial^2}{\partial \varphi^2} + i\hbar^2 \frac{\partial}{\partial \varphi} \\
&= -\hbar^2 \frac{\partial^2}{\partial \theta^2} - \hbar^2 \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \theta} - \hbar^2 \left(1 + \frac{\cos^2 \theta}{\sin^2 \theta} \right) \frac{\partial^2}{\partial \varphi^2} \\
&\quad + i\hbar^2 \left(-1 - \frac{\cos^2 \theta}{\sin^2 \theta} + 1 + \frac{\cos^2 \theta}{\sin^2 \theta} \right) \frac{\partial}{\partial \varphi} \\
&= -\hbar^2 \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right)
\end{aligned}$$

This last equation establishes the relationship between the spherical harmonics and the angular momentum states, because the Laplace equation in spherical coordinates is

$$\begin{aligned}
\nabla^2 &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \\
&= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \hat{\mathbf{L}}^2
\end{aligned}$$

and we know that the general solution for $f(r, \theta, \varphi)$ is given in terms of spherical harmonics,

$$f(r, \theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l A_l(r) Y_m^l(\theta, \varphi)$$

where the spherical harmonics satisfy

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} Y_m^l(\theta, \varphi) \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} Y_m^l(\theta, \varphi) + l(l+1) Y_m^l(\theta, \varphi) = 0$$

for integer l and $m = -l, -l+1, \dots, +l$, while the eigenstates of $\hat{\mathbf{L}}^2$ satisfy precisely the same equation,

$$\langle \mathbf{x} | \hat{\mathbf{L}}^2 | l, m \rangle = l(l+1) \hbar^2 \langle \mathbf{x} | l, m \rangle$$

with $\hat{\mathbf{L}}^2$ given above. This shows that orbital angular momentum only describes integer j states.

4 Spherical harmonics

We can now use the quantum formalism to find the spherical harmonics, $Y_m^l(\theta, \varphi) = \langle \theta, \varphi | l, m \rangle$. For any state $|\alpha\rangle$, we know the effect of \hat{L}_z is given by

$$\begin{aligned} \langle \theta, \varphi | \hat{L}_z | \alpha \rangle &= -i\hbar \frac{\partial}{\partial \varphi} \langle \theta, \varphi | \alpha \rangle \\ \langle \theta, \varphi | \hat{L}_z | l, m \rangle &= m\hbar \langle \theta, \varphi | l, m \rangle \\ \langle \theta, \varphi | \hat{L}_z | l, m \rangle &= -i\hbar \frac{\partial}{\partial \varphi} \langle \theta, \varphi | l, m \rangle \end{aligned}$$

so for an eigenstate,

$$-i\hbar \frac{\partial}{\partial \varphi} \langle \theta, \varphi | l, m \rangle = m\hbar \langle \theta, \varphi | l, m \rangle$$

This is trivially integrated to give

$$\langle \theta, \varphi | l, m \rangle = e^{im\varphi} \langle \theta, \varphi | l \rangle$$

Furthermore, we know that the raising operator will annihilate the state with the highest value of m ,

$$\hat{L}_+ | l, m = l \rangle = 0$$

In a coordinate basis, this translates to a differential equation,

$$\begin{aligned} 0 &= \langle \theta, \varphi | \hat{L}_+ | l, l \rangle \\ &= \hbar e^{il\varphi} \left(\frac{\partial}{\partial \theta} + i \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \right) e^{il\varphi} \langle \theta, \varphi | l, l \rangle \\ &= \hbar e^{il\varphi} \left(\frac{\partial}{\partial \theta} + i \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \right) e^{il\varphi} \langle \theta, \varphi | l \rangle \end{aligned}$$

Setting $\langle \mathbf{x} | l \rangle = f_l(\theta)$, we have

$$0 = \sin \theta \frac{\partial f_l}{\partial \theta} - l \cos \theta f_l$$

This is solved by $f_l = \sin^l \theta$, so we have, for $m = l$

$$Y_{l, l}^l(\theta, \varphi) = A_l e^{il\varphi} \sin^l \theta$$

Now we can find all other $Y^l_m(\theta, \varphi)$ by acting with the lowering operator,

$$\langle \theta, \varphi | \hat{L}_- | l, m \rangle = \sqrt{l(l+1) - m(m-1)} \hbar \langle \theta, \varphi | l, m-1 \rangle$$

Inserting the coordinate expression for $\langle \theta, \varphi | \hat{L}_- | l, m \rangle$ and solving for the next lower state, we have

$$\begin{aligned} \langle \theta, \varphi | l, m-1 \rangle &= \frac{e^{-i\varphi}}{\sqrt{l(l+1) - m(m-1)}} \left(-\frac{\partial}{\partial \theta} + i \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \varphi} \right) \langle \theta, \varphi | l, m \rangle \\ &= -\frac{e^{-i\varphi} e^{im\varphi}}{\sqrt{l(l+1) - m(m-1)}} \left(\frac{\partial}{\partial \theta} + m \frac{\cos \theta}{\sin \theta} \right) \langle \theta | l, m \rangle \end{aligned}$$

thereby defining all $Y^l_m(\theta, \varphi)$ recursively.