参考 **具体的なラプラシアンの計算**

$\frac{\partial^2 \varphi}{\partial x^2}$ は、

$$\frac{\partial^2 \varphi}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial \varphi}{\partial x}$$

$$= \frac{\partial \frac{\partial \varphi}{\partial x}}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial \frac{\partial \varphi}{\partial x}}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial \frac{\partial \varphi}{\partial x}}{\partial \phi}\frac{\partial \phi}{\partial x}$$

$$= \frac{\partial(\sin\theta\cos\phi\frac{\partial \varphi}{\partial r} + \frac{1}{r}\cos\theta\cos\phi\frac{\partial \varphi}{\partial \theta} - \frac{1}{r}\frac{\sin\phi}{\sin\theta}\frac{\partial \varphi}{\partial \phi})}{\partial r}\sin\theta\cos\phi$$

$$+ \frac{\partial(\sin\theta\cos\phi\frac{\partial \varphi}{\partial r} + \frac{1}{r}\cos\theta\cos\phi\frac{\partial \varphi}{\partial \theta} - \frac{1}{r}\frac{\sin\phi}{\sin\theta}\frac{\partial \varphi}{\partial \phi})}{\partial \theta}\frac{\cos\theta\cos\phi}{r}$$

$$- \frac{\partial(\sin\theta\cos\phi\frac{\partial \varphi}{\partial r} + \frac{1}{r}\cos\theta\cos\phi\frac{\partial \varphi}{\partial \theta} - \frac{1}{r}\frac{\sin\phi}{\sin\theta}\frac{\partial \varphi}{\partial \phi})}{\partial \phi}\frac{\sin\phi}{r\sin\theta}$$

$$= \left[\sin\theta\cos\phi\frac{\partial^2 \varphi}{\partial r^2} + \cos\theta\cos\phi\left(-\frac{1}{r^2}\frac{\partial \varphi}{\partial \theta} + \frac{1}{r}\frac{\partial^2 \varphi}{\partial \theta \partial r}\right)\right.$$

$$\left. - \frac{\sin\phi}{\sin\theta}\left(-\frac{1}{r^2}\frac{\partial \varphi}{\partial \phi} + \frac{1}{r}\frac{\partial^2 \varphi}{\partial \phi \partial r}\right)\right]\sin\theta\cos\phi$$

$$+ \left[\cos\phi\left(\cos\theta\frac{\partial \varphi}{\partial r} + \sin\theta\frac{\partial^2 \varphi}{\partial r \partial \theta}\right) + \frac{1}{r}\cos\phi\left(-\sin\theta\frac{\partial \varphi}{\partial \theta} + \cos\theta\frac{\partial^2 \varphi}{\partial^2 \theta}\right)\right.$$

$$\left. - \frac{1}{r}\sin\phi\left(-\frac{\cos\theta}{\sin^2\theta}\frac{\partial \varphi}{\partial \phi} + \frac{1}{\sin\theta}\frac{\partial^2 \varphi}{\partial \phi \partial \theta}\right)\right]\frac{\cos\theta\cos\phi}{r}$$

$$+ \left[-\sin\theta\left(-\sin\phi\frac{\partial \varphi}{\partial r} + \cos\phi\frac{\partial^2 \varphi}{\partial r \partial \phi}\right) - \frac{1}{r}\cos\theta\left(-\sin\phi\frac{\partial \varphi}{\partial \theta} + \cos\phi\frac{\partial^2 \varphi}{\partial \theta \partial \phi}\right)\right.$$

$$\left. + \frac{1}{r}\frac{1}{\sin\theta}\left(\cos\phi\frac{\partial \varphi}{\partial \phi} + \sin\phi\frac{\partial^2 \varphi}{\partial \phi^2}\right)\right]\frac{\sin\phi}{r\sin\theta}$$

$$= \sin^2\theta\cos^2\phi\frac{\partial^2 \varphi}{\partial r^2} + \left(\cos^2\theta\cos^2\phi + \sin^2\phi\right)\frac{1}{r}\frac{\partial \varphi}{\partial r}$$

$$+ \frac{1}{r^2}\left[\left(-2\cos\theta\sin\theta\cos^2\phi + \frac{\cos\theta}{\sin\theta}\sin^2\phi\right)\frac{\partial \varphi}{\partial \theta} + \cos^2\theta\cos^2\phi\frac{\partial^2 \varphi}{\partial \theta^2}\right.$$

$$\left. + \left(\sin\phi\cos\phi + \frac{\sin\phi\cos\phi\cos^2\theta}{\sin^2\theta} + \frac{\cos\phi\sin\phi}{\sin^2\theta}\right)\frac{\partial \varphi}{\partial \phi} + \frac{\sin^2\phi}{\sin^2\theta}\frac{\partial^2 \varphi}{\partial \phi^2}\right]$$

$$+ \frac{2}{r}\left[\cos\theta\sin\theta\cos^2\phi\frac{\partial^2 \varphi}{\partial r \partial \theta} - \sin\phi\cos\phi\frac{\partial^2 \varphi}{\partial r \partial \phi} - \frac{1}{r}\frac{\cos\theta}{\sin\theta}\sin\phi\cos\phi\frac{\partial^2 \varphi}{\partial \theta \partial \phi}\right]$$

$$\tag{9.20}$$

となります。同様にして $\frac{\partial^2 \varphi}{\partial y^2}$ は、

$$\frac{\partial^2 \varphi}{\partial y^2} = \frac{\partial}{\partial y} \frac{\partial \varphi}{\partial y}$$

$$= \frac{\partial \frac{\partial \varphi}{\partial y}}{\partial r} \frac{\partial r}{\partial y} + \frac{\partial \frac{\partial \varphi}{\partial y}}{\partial \theta} \frac{\partial \theta}{\partial y} + \frac{\partial \frac{\partial \varphi}{\partial y}}{\partial \phi} \frac{\partial \phi}{\partial y}$$

$$= \frac{\partial \left(\sin\theta \sin\phi \frac{\partial \varphi}{\partial r} + \frac{1}{r} \cos\theta \sin\phi \frac{\partial \varphi}{\partial \theta} + \frac{1}{r} \frac{\cos\phi}{\sin\theta} \frac{\partial \varphi}{\partial \phi} \right)}{\partial r} \sin\theta \sin\phi$$

$$+ \frac{\partial \left(\sin\theta \sin\phi \frac{\partial \varphi}{\partial r} + \frac{1}{r} \cos\theta \sin\phi \frac{\partial \varphi}{\partial \theta} + \frac{1}{r} \frac{\cos\phi}{\sin\theta} \frac{\partial \varphi}{\partial \phi} \right)}{\partial \theta} \frac{\cos\theta \sin\phi}{r}$$

$$+ \frac{\partial \left(\sin\theta \sin\phi \frac{\partial \varphi}{\partial r} + \frac{1}{r} \cos\theta \sin\phi \frac{\partial \varphi}{\partial \theta} + \frac{1}{r} \frac{\cos\phi}{\sin\theta} \frac{\partial \varphi}{\partial \phi} \right)}{\partial \phi} \frac{\cos\phi}{r \sin\theta}$$

$$= \left[\sin\theta \sin\phi \frac{\partial^2 \varphi}{\partial r^2} + \cos\theta \sin\phi \left(-\frac{1}{r^2} \frac{\partial \varphi}{\partial \theta} + \frac{1}{r} \frac{\partial^2 \varphi}{\partial \theta \partial r} \right) \right.$$

$$\left. + \frac{\cos\phi}{\sin\theta} \left(-\frac{1}{r^2} \frac{\partial \varphi}{\partial \phi} + \frac{1}{r} \frac{\partial^2 \varphi}{\partial \phi \partial r} \right) \right] \sin\theta \sin\phi$$

$$+ \left[\sin\phi \left(\cos\theta \frac{\partial \varphi}{\partial r} + \sin\theta \frac{\partial^2 \varphi}{\partial r \partial \theta} \right) + \frac{1}{r} \sin\phi \left(-\sin\theta \frac{\partial \varphi}{\partial \theta} + \cos\theta \frac{\partial^2 \varphi}{\partial \theta^2} \right) \right.$$

$$\left. + \frac{1}{r} \cos\phi \left(-\frac{\cos\theta}{\sin^2\theta} \frac{\partial \varphi}{\partial \phi} + \frac{1}{\sin\theta} \frac{\partial^2 \varphi}{\partial \phi \partial \theta} \right) \right] \frac{\cos\theta \sin\phi}{r}$$

$$+ \left[\sin\theta \left(\cos\phi \frac{\partial \varphi}{\partial r} + \sin\phi \frac{\partial^2 \varphi}{\partial r \partial \phi} \right) + \frac{1}{r} \cos\theta \left(\cos\phi \frac{\partial \varphi}{\partial \theta} + \sin\phi \frac{\partial^2 \varphi}{\partial \theta \partial \phi} \right) \right.$$

$$\left. + \frac{1}{r} \frac{1}{\sin\theta} \left(-\sin\phi \frac{\partial \varphi}{\partial \phi} + \cos\phi \frac{\partial^2 \varphi}{\partial \phi^2} \right) \right] \frac{\cos\phi}{r \sin\theta}$$

$$= \sin^2\theta \sin^2\phi \frac{\partial^2 \varphi}{\partial r^2} + (\cos^2\theta \sin^2\phi + \cos^2\phi) \frac{1}{r} \frac{\partial \varphi}{\partial r}$$

$$+ \frac{1}{r^2} \left[\left(-2\cos\theta \sin\theta \sin^2\phi + \frac{\cos\theta}{\sin\theta} \cos^2\phi \right) \frac{\partial \varphi}{\partial \theta} + \cos^2\theta \sin^2\phi \frac{\partial^2 \varphi}{\partial \theta^2} \right.$$

$$\left. - \left(\cos\phi \sin\phi + \frac{\cos\phi \sin\phi \cos^2\theta}{\sin^2\theta} + \frac{\sin\phi \cos\phi}{\sin^2\theta} \right) \frac{\partial \varphi}{\partial \phi} + \frac{\cos^2\phi}{\sin^2\theta} \frac{\partial^2 \varphi}{\partial \phi^2} \right]$$

$$+ \frac{2}{r} \left[\cos\theta \sin\theta \sin^2\phi \frac{\partial^2 \varphi}{\partial r \partial \theta} + \sin\phi \cos\phi \frac{\partial^2 \varphi}{\partial r \partial \phi} + \frac{1}{r} \frac{\cos\theta}{\sin\theta} \sin\phi \cos\phi \frac{\partial^2 \varphi}{\partial \theta \partial \phi} \right]$$

$$(9.21)$$

となります。同様にして $\frac{\partial^2 \varphi}{\partial z^2}$ は、

$$\frac{\partial^2 \varphi}{\partial z^2} = \frac{\partial}{\partial z}\frac{\partial \varphi}{\partial z}$$

$$= \frac{\partial \frac{\partial \varphi}{\partial z}}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial \frac{\partial \varphi}{\partial z}}{\partial \theta}\frac{\partial \theta}{\partial z} + \frac{\partial \frac{\partial \varphi}{\partial z}}{\partial \phi}\frac{\partial \phi}{\partial z}$$

$$= \frac{\partial \left(\cos\theta \frac{\partial \varphi}{\partial r} - \frac{1}{r}\sin\theta \frac{\partial \varphi}{\partial \theta}\right)}{\partial r}\cos\theta - \frac{\partial \left(\cos\theta \frac{\partial \varphi}{\partial r} - \frac{1}{r}\sin\theta \frac{\partial \varphi}{\partial \theta}\right)}{\partial \theta}\frac{\sin\theta}{r}$$

$$= \left[\cos\theta \frac{\partial^2 \varphi}{\partial r^2} - \sin\theta\left(-\frac{1}{r^2}\frac{\partial \varphi}{\partial \theta} + \frac{1}{r}\frac{\partial^2 \varphi}{\partial \theta \partial r}\right)\right]\cos\theta$$

$$\quad + \left[\left(\sin\theta \frac{\partial \varphi}{\partial r} - \cos\theta \frac{\partial^2 \varphi}{\partial r \partial \theta}\right) + \frac{1}{r}\left(\cos\theta \frac{\partial \varphi}{\partial \theta} + \sin\theta \frac{\partial^2 \varphi}{\partial \theta^2}\right)\right]\frac{\sin\theta}{r}$$

$$= \cos^2\theta \frac{\partial^2 \varphi}{\partial r^2} + \sin^2\theta \frac{1}{r}\frac{\partial \varphi}{\partial r} + \frac{1}{r^2}\left[2\sin\theta\cos\theta \frac{\partial \varphi}{\partial \theta} + \sin^2\theta \frac{\partial^2 \varphi}{\partial \theta^2}\right] - \frac{2}{r}\cos\theta\,\sin\theta\,\frac{\partial^2 \varphi}{\partial r \partial \theta}$$

$$\tag{9.22}$$

となります。これで直交座標 x, y, z 座標での2階微分を極座標 r, θ, ϕ で表すことができたので、直交座標で表されたラプラシアンに φ をかけた式を極座標で表すと、式 (9.20)、(9.21)、(9.22) を使い、微分の項ごとにまとめていくと、以下のようになります。

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2}$$

$$= \left(\sin^2\theta\cos^2\phi + \sin^2\theta\sin^2\phi + \cos^2\theta\right)\frac{\partial^2 \varphi}{\partial r^2}$$

$$+ \left(\cos^2\theta\cos^2\phi + \sin^2\phi + \cos^2\theta\sin^2\phi + \cos^2\phi + \sin^2\theta\right)\frac{1}{r}\frac{\partial \varphi}{\partial r}$$

$$+ \left(\sin\phi\cos\phi + \frac{\sin\phi\cos\phi\cos^2\theta}{\sin^2\theta} + \frac{\cos\phi\sin\phi}{\sin^2\theta}\right.$$

$$\quad \left. - \sin\phi\cos\phi - \frac{\sin\phi\cos\phi\cos^2\theta}{\sin^2\theta} - \frac{\cos\phi\sin\phi}{\sin^2\theta}\right)\frac{1}{r^2}\frac{\partial \varphi}{\partial \phi}$$

$$+ \left(\frac{\sin^2\phi}{\sin^2\theta} + \frac{\cos^2\phi}{\sin^2\theta}\right)\frac{1}{r^2}\frac{\partial^2 \varphi}{\partial \phi^2}$$

$$+ \left(-2\cos\theta\sin\theta\cos^2\phi + \frac{\cos\theta}{\sin\theta}\sin^2\phi\right.$$

$$\quad \left. -2\cos\theta\sin\theta\sin^2\phi + \frac{\cos\theta}{\sin\theta}\cos^2\phi + 2\sin\theta\cos\theta\right)\frac{1}{r^2}\frac{\partial \varphi}{\partial \theta}$$

$$+ \left(\cos^2\theta\cos^2\phi + \cos^2\theta\sin^2\phi + \sin^2\theta\right)\frac{1}{r^2}\frac{\partial^2 \varphi}{\partial \theta^2}$$

$$+ \frac{2}{r}\left[\left(\cos\theta\sin\theta\cos^2\phi + \cos\theta\sin\theta\sin^2\phi - \cos\theta\sin\theta\right)\frac{\partial^2 \varphi}{\partial r \partial \theta}\right.$$

$$\quad \left. + \left(-\sin\phi\cos\phi + \sin\phi\cos\phi\right)\frac{\partial^2 \varphi}{\partial r \partial \phi} + \left(-\frac{1}{r}\frac{\cos\theta}{\sin\theta}\sin\phi\cos\phi + \frac{1}{r}\frac{\cos\theta}{\sin\theta}\sin\phi\cos\phi\right)\frac{\partial^2 \varphi}{\partial \theta \partial \phi}\right]$$

$$= \frac{\partial^2 \varphi}{\partial r^2} + \frac{2}{r}\frac{\partial \varphi}{\partial r} + \frac{1}{r^2}\left(\frac{\cos\theta}{\sin\theta}\frac{\partial \varphi}{\partial \theta} + \frac{\partial^2 \varphi}{\partial \theta^2} + \frac{1}{\sin^2\theta}\frac{\partial^2 \varphi}{\partial \phi^2}\right)$$

$$\tag{9.23}$$

つまり、極座標で表されたラプラシアンに φ をかけた式 $\Delta\varphi$ は、

$$\Delta\varphi = \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2} = \frac{\partial^2\varphi}{\partial r^2} + \frac{2}{r}\frac{\partial\varphi}{\partial r} + \frac{1}{r^2}\left(\frac{\cos\theta}{\sin\theta}\frac{\partial\varphi}{\partial\theta} + \frac{\partial^2\varphi}{\partial\theta^2} + \frac{1}{\sin^2\theta}\frac{\partial^2\varphi}{\partial\phi^2}\right)$$

(9.24)

となります。また、

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\varphi}{\partial\theta}) = \frac{1}{\sin\theta}(\cos\theta\frac{\partial\varphi}{\partial\theta} + \sin\theta\frac{\partial^2\varphi}{\partial\theta^2})$$
$$= \frac{\cos\theta}{\sin\theta}\frac{\partial\varphi}{\partial\theta} + \frac{\partial^2\varphi}{\partial\theta^2}$$

(9.25)

なので、極座標で表されたラプラシアン φ にをかけた $\Delta\varphi$ を、

$$\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2} = \frac{\partial^2\varphi}{\partial r^2} + \frac{2}{r}\frac{\partial\varphi}{\partial r} + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\varphi}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2\varphi}{\partial\phi^2}\right)$$

(9.26)

と書くこともあります。これで式（9.17）が得られました。

❖球対称ポテンシャルにおける極座標シュレーディンガー方程式の変数分離

この極座標で表されたシュレーディンガー方程式は一般には解くことは困難です。しかし、第5章で見たように原子、原子核などさまざまな場合において、ポテンシャルは角度依存性がなく、**球対称** $V(r)$ でした。実はポテンシャルが球対称 $V(r)$ ならば、本書で何度も出てきた変数分離法によって簡単になることが知られています。そこで、本書ではポテンシャルは球対称 $V(r)$ である場合のみを考えましょう。

極座標シュレーディンガー方程式でポテンシャルを球対称 $V(r)$ と置いた式、

$$-\frac{\hbar^2}{2m}\left[\frac{d^2\varphi}{dr^2} + \frac{2}{r}\frac{d\varphi}{dr} + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\varphi}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2\varphi}{\partial\phi^2}\right)\right] + V(r)\varphi = E\varphi$$

(9.27)

第9章 3次元シュレーディンガー方程式の解 I（直交座標及びs波の場合）