total variation $dV = \nabla V \cdot d\mathbf{r} = -\mathbf{F} \cdot d\mathbf{r}$ is the work done against the force along the path $d\mathbf{r}$, we recognize the physical meaning of the potential (difference) as work and energy. Moreover, in a sum of path increments the intermediate points cancel,

$$\left[V(\mathbf{r} + d\mathbf{r}_1 + d\mathbf{r}_2) - V(\mathbf{r} + d\mathbf{r}_1)\right] + \left[V(\mathbf{r} + d\mathbf{r}_1) - V(\mathbf{r})\right] = V(\mathbf{r} + d\mathbf{r}_2 + d\mathbf{r}_1) - V(\mathbf{r}),$$

so the integrated work along some path from an initial point $\mathbf{r}_i$ to a final point $\mathbf{r}$ is given by the potential difference $V(\mathbf{r}) - V(\mathbf{r}_i)$ at the endpoints of the path. Therefore, such forces are especially simple and well behaved: They are called **conservative**. When there is loss of energy due to friction along the path or some other dissipation, the work will depend on the path, and such forces cannot be conservative: No potential exists. We discuss conservative forces in more detail in Section 1.13.

Example 1.6.1 THE GRADIENT OF A POTENTIAL $V(r)$

Let us calculate the gradient of $V(r) = V(\sqrt{x^2 + y^2 + z^2})$, so

$$\nabla V(r) = \hat{\mathbf{x}}\frac{\partial V(r)}{\partial x} + \hat{\mathbf{y}}\frac{\partial V(r)}{\partial y} + \hat{\mathbf{z}}\frac{\partial V(r)}{\partial z}.$$

Now, $V(r)$ depends on x through the dependence of r on x. Therefore[14]

$$\frac{\partial V(r)}{\partial x} = \frac{dV(r)}{dr} \cdot \frac{\partial r}{\partial x}.$$

From r as a function of x, y, z,

$$\frac{\partial r}{\partial x} = \frac{\partial (x^2 + y^2 + z^2)^{1/2}}{\partial x} = \frac{x}{(x^2 + y^2 + z^2)^{1/2}} = \frac{x}{r}.$$

Therefore

$$\frac{\partial V(r)}{\partial x} = \frac{dV(r)}{dr} \cdot \frac{x}{r}.$$

Permuting coordinates ($x \to y, y \to z, z \to x$) to obtain the y and z derivatives, we get

$$\boxed{\begin{aligned}\nabla V(r) &= (\hat{\mathbf{x}}x + \hat{\mathbf{y}}y + \hat{\mathbf{z}}z)\frac{1}{r}\frac{dV}{dr}\\ &= \frac{\mathbf{r}}{r}\frac{dV}{dr} = \hat{\mathbf{r}}\frac{dV}{dr}.\end{aligned}}$$

Here $\hat{\mathbf{r}}$ is a unit vector $(\mathbf{r}/r)$ in the **positive** radial direction. The gradient of a function of r is a vector in the (positive or negative) radial direction. In Section 2.5, $\hat{\mathbf{r}}$ is seen as one of the three orthonormal unit vectors of spherical polar coordinates and $\hat{\mathbf{r}}\partial/\partial r$ as the radial component of ∇. ■

[14]This is a special case of the **chain rule** of partial differentiation:

$$\frac{\partial V(r, \theta, \varphi)}{\partial x} = \frac{\partial V}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial V}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial V}{\partial \varphi}\frac{\partial \varphi}{\partial x},$$

where $\partial V/\partial \theta = \partial V/\partial \varphi = 0$, $\partial V/\partial r \to dV/dr$.

A Geometrical Interpretation

One immediate application of $\nabla\varphi$ is to dot it into an increment of length

$$d\mathbf{r} = \hat{\mathbf{x}}\,dx + \hat{\mathbf{y}}\,dy + \hat{\mathbf{z}}\,dz.$$

Thus we obtain

$$\nabla\varphi \cdot d\mathbf{r} = \frac{\partial\varphi}{\partial x}dx + \frac{\partial\varphi}{\partial y}dy + \frac{\partial\varphi}{\partial z}dz = d\varphi,$$

the change in the scalar function φ corresponding to a change in position $d\mathbf{r}$. Now consider P and Q to be two points on a surface $\varphi(x, y, z) = C$, a constant. These points are chosen so that Q is a distance $d\mathbf{r}$ from P. Then, moving from P to Q, the change in $\varphi(x, y, z) = C$ is given by

$$d\varphi = (\nabla\varphi) \cdot d\mathbf{r} = 0 \tag{1.63}$$

since we stay on the surface $\varphi(x, y, z) = C$. This shows that $\nabla\varphi$ is perpendicular to $d\mathbf{r}$. Since $d\mathbf{r}$ may have any direction from P **as long as it stays in the surface** of constant φ, point Q being restricted to the surface but having arbitrary direction, $\nabla\varphi$ is seen as normal to the surface $\varphi = \text{constant}$ (Fig. 1.19).

If we now permit $d\mathbf{r}$ to take us from one surface $\varphi = C_1$ to an adjacent surface $\varphi = C_2$ (Fig. 1.20),

$$d\varphi = C_1 - C_2 = \Delta C = (\nabla\varphi) \cdot d\mathbf{r}. \tag{1.64}$$

For a given $d\varphi$, $|d\mathbf{r}|$ is a minimum when it is chosen parallel to $\nabla\varphi$ ($\cos\theta = 1$); or, for a given $|d\mathbf{r}|$, the change in the scalar function φ is maximized by choosing $d\mathbf{r}$ parallel to

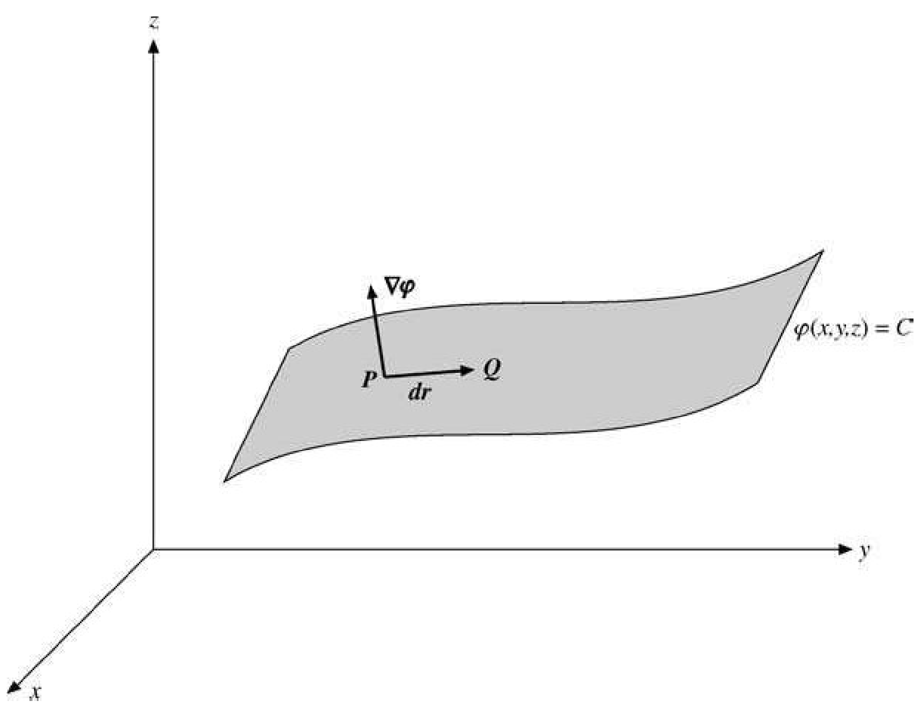

FIGURE 1.19 The length increment $d\mathbf{r}$ has to stay on the surface $\varphi = C$.

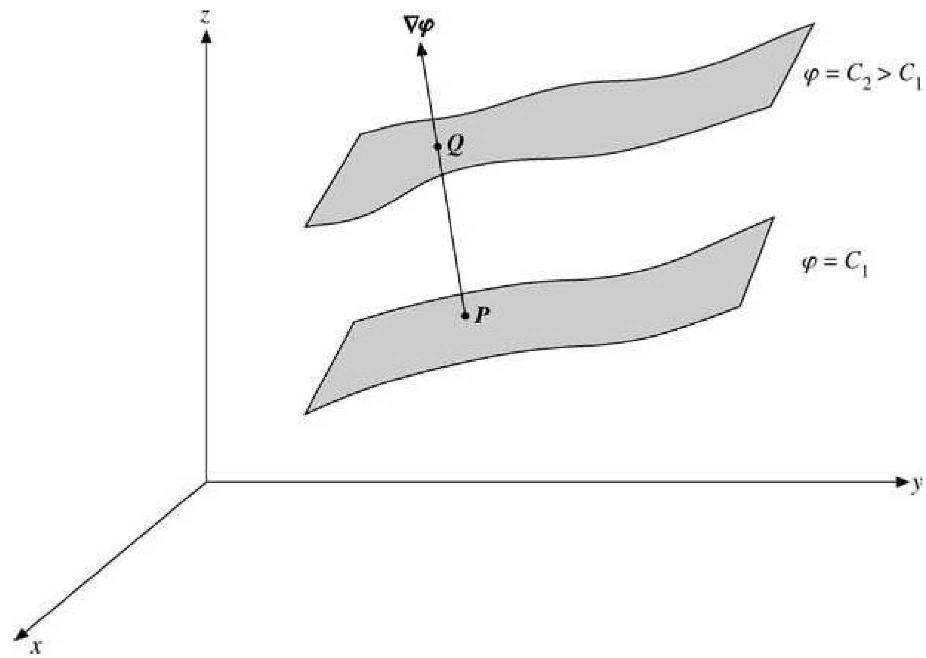

FIGURE 1.20 Gradient.

$\nabla\varphi$. **This identifies $\nabla\varphi$ as a vector having the direction of the maximum space rate of change of** φ, an identification that will be useful in Chapter 2 when we consider non-Cartesian coordinate systems. This identification of $\nabla\varphi$ may also be developed by using the calculus of variations subject to a constraint, Exercise 17.6.9.

Example 1.6.2 FORCE AS GRADIENT OF A POTENTIAL

As a specific example of the foregoing, and as an extension of Example 1.6.1, we consider the surfaces consisting of concentric spherical shells, Fig. 1.21. We have

$$\varphi(x, y, z) = \left(x^2 + y^2 + z^2\right)^{1/2} = r = C,$$

where r is the radius, equal to C, our constant. $\Delta C = \Delta\varphi = \Delta r$, the distance between two shells. From Example 1.6.1

$$\nabla\varphi(r) = \hat{\mathbf{r}}\frac{d\varphi(r)}{dr} = \hat{\mathbf{r}}.$$

The gradient is in the radial direction and is normal to the spherical surface $\varphi = C$. ■

Example 1.6.3 INTEGRATION BY PARTS OF GRADIENT

Let us prove the formula $\int \mathbf{A}(\mathbf{r}) \cdot \nabla f(\mathbf{r})\, d^3r = -\int f(\mathbf{r})\nabla \cdot \mathbf{A}(\mathbf{r})\, d^3r$, where $\mathbf{A}$ or f or both vanish at infinity so that the integrated parts vanish. This condition is satisfied if, for example, $\mathbf{A}$ is the electromagnetic vector potential and f is a bound-state wave function $\psi(\mathbf{r})$.

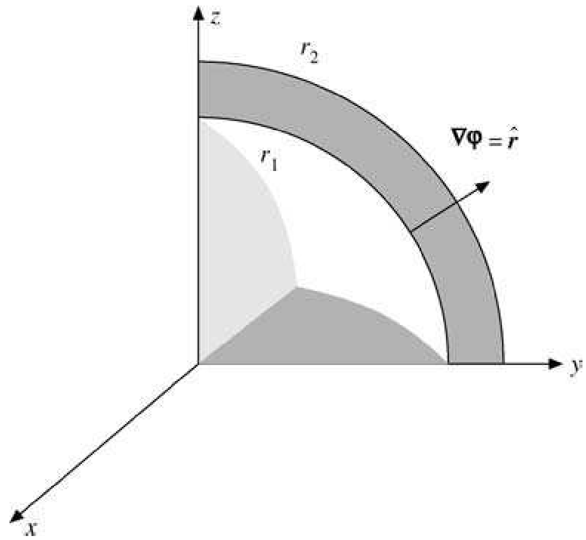

FIGURE 1.21 Gradient for $\varphi(x, y, z) = (x^2 + y^2 + z^2)^{1/2}$, spherical shells: $(x_2^2 + y_2^2 + z_2^2)^{1/2} = r_2 = C_2$, $(x_1^2 + y_1^2 + z_1^2)^{1/2} = r_1 = C_1$.

Writing the inner product in Cartesian coordinates, integrating each one-dimensional integral by parts, and dropping the integrated terms, we obtain

$$\int \mathbf{A}(\mathbf{r}) \cdot \nabla f(\mathbf{r})\, d^3r = \iint \left[A_x f|_{x=-\infty}^{\infty} - \int f \frac{\partial A_x}{\partial x} dx \right] dy\, dz + \cdots$$
$$= -\iiint f \frac{\partial A_x}{\partial x} dx\, dy\, dz - \iiint f \frac{\partial A_y}{\partial y} dy\, dx\, dz - \iiint f \frac{\partial A_z}{\partial z} dz\, dx\, dy$$
$$= -\int f(\mathbf{r}) \nabla \cdot \mathbf{A}(\mathbf{r})\, d^3r.$$

If $\mathbf{A} = e^{ikz}\hat{\mathbf{e}}$ describes an outgoing photon in the direction of the constant polarization unit vector $\hat{\mathbf{e}}$ and $f = \psi(\mathbf{r})$ is an exponentially decaying bound-state wave function, then

$$\int e^{ikz}\hat{\mathbf{e}} \cdot \nabla \psi(\mathbf{r})\, d^3r = -e_z \int \psi(\mathbf{r}) \frac{de^{ikz}}{dz} d^3r = -ike_z \int \psi(\mathbf{r}) e^{ikz}\, d^3r,$$

because only the z-component of the gradient contributes. ■

Exercises

1.6.1 If $S(x, y, z) = (x^2 + y^2 + z^2)^{-3/2}$, find

(a) ∇S at the point $(1, 2, 3)$;
(b) the magnitude of the gradient of S, $|\nabla S|$ at $(1, 2, 3)$; and
(c) the direction cosines of ∇S at $(1, 2, 3)$.