1
Symmetry and physics

1.1 Introduction

The application of *group theory* to study physical problems and their solutions provides a formal method for exploiting the simplifications made possible by the presence of symmetry. Often the symmetry that is readily apparent is the symmetry of the system/object of interest, such as the three-fold axial symmetry of an NH_3 molecule. The symmetry exploited in actual analysis is the symmetry of the Hamiltonian. When alluding to symmetry we usually include geometrical, time-reversal symmetry, and symmetry associated with the exchange of identical particles.

Conservation laws of physics are rooted in the symmetries of the underlying space and time. The most common physical laws we are familiar with are actually manifestations of some universal symmetries. For example, the homogeneity and isotropy of space lead to the conservation of linear and angular momentum, respectively, while the homogeneity of time leads to the conservation of energy. Such laws have come to be known as universal conservation laws. As we will delineate in a later chapter, the relation between these classical symmetries and corresponding conserved quantities is beautifully cast in a theorem due to Emmy Noether.

At the day-to-day working level of the physicist dealing with quantum mechanics, the application of symmetry restrictions leads to familiar results, such as selection rules and characteristic transformations of eigenfunctions when acted upon by symmetry operations that leave the Hamiltonian of the system invariant.

In a similar manner, we expect that when a physical system/object is endowed with special symmetries, these symmetries forge conservation relations that ultimately determine its physical properties. Traditionally, the derivation of the physical states of a system has been performed without invoking the symmetry properties, however, the advantage of taking account of symmetry aspects is that it results in great simplification of the underlying analysis, and it provides powerful insight into the nature and the physics of the system. The mathematical framework that translates these symmetries into suitable mathematical relations is found in the theory of groups and group representations. This is the subject we will try to elucidate throughout the chapters of this book.

Let us begin with a tour de force, exploring the merits of invoking symmetry aspects pertinent to familiar but simple problems. We start by reminding ourselves of the trivial example of using symmetry, or asymmetry, to simplify the evaluation of an integral.

Consider

$$\int_{-b}^{+b} \sin x \, dx = 0.$$

We *know* this to be true because $\sin x$ is an odd function; $\sin(-x) = -\sin(x)$. In evaluating this integral, we have taken advantage of the asymmetry of its integrand. In order to cast this problem in the language of symmetry we introduce two mathematical operations: I, which we will identify later with the operation of inversion, and which, for now, changes the sign of the argument of a function, i.e. $I\,f(x) = f(-x)$; and E, which is an identity operation, $E\,f(x) = f(x)$. This allows us to write

$$\int_{-b}^{+b} \sin x \, dx = \int_{0}^{b} (E + I) \sin(x) \, dx = \int_{0}^{b} \big(1 + (-1)\big) \sin(x) \, dx = 0.$$

Figure 1.1 shows schematically the plane of integration, with $\oplus$ and $\ominus$ indicating the sign of the function $\sin x$.

We may introduce a more complicated integrand function $f(x, y)$, and carry the integration over the equilateral triangular area shown in Figure 1.2.

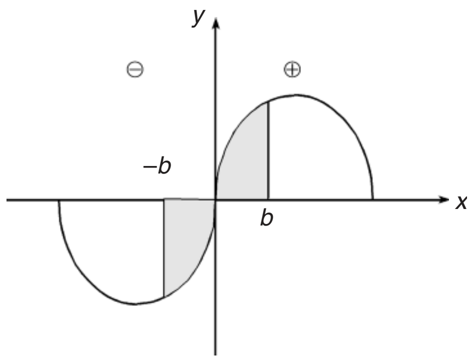

Fig. 1.1. The asymmetric function sin x.

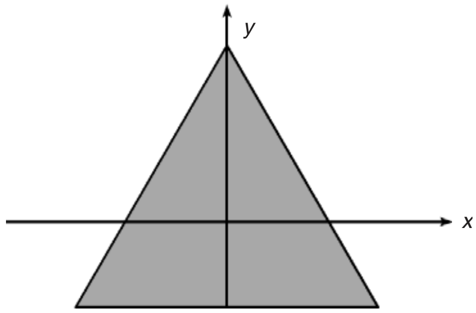

Fig. 1.2. Integration domain.

Making use of the 3-fold symmetry of the triangle, which includes rotations by multiples of $2\pi/3$, as well as reflections shown in Figure 1.3, we write the integral in the form

$$\int_{\text{triangle}} f(x,y)\,dx\,dy = \int_{\text{wedge}} \left(E + O_{(2\pi/3)} + O_{(4\pi/3)} + \sigma_1 + \sigma_2 + \sigma_3\right) \times f(x,y)\,dx\,dy,$$

where the Os represent counterclockwise rotations by the angle specified in the suffix, and the σs are defined in Figure 1.3. Now, if the function $f(x,y)$ possesses a symmetry which can be associated with that of the triangle, as for example shown in Figure 1.4, the integral vanishes.

Later, we will see how to reach similar conclusions in the case of selection rules, for example, where the situation may be much more complicated.

Next, we present a simple example to demonstrate how to invoke symmetry to simplify the solution of dynamical problems. We consider a system of two masses and three springs as illustrated in Figure 1.5. Assume both masses to be equal to m and that all springs have the force constant κ. In that case, the Hamiltonian, which is the

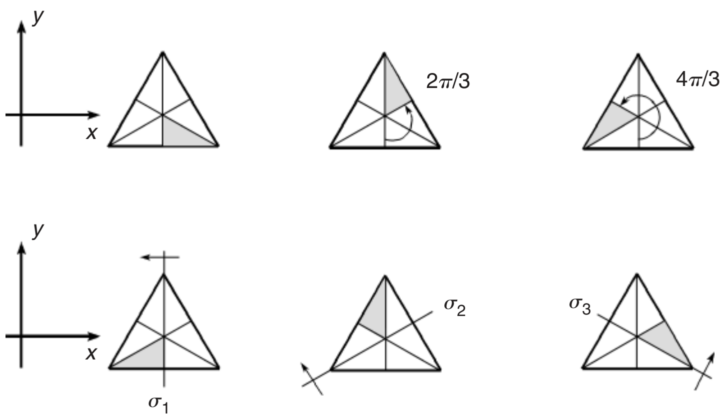

Fig. 1.3. Symmetry operations of an equilateral triangle.

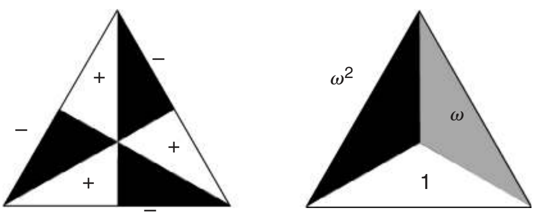

Fig. 1.4. Some possible symmetries of $f(x,y)$ on an equilateral triangle.

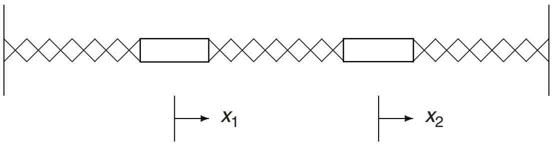

Fig. 1.5. A two-mass system with inversion symmetry about the center point.

total energy of the system,

$$\mathcal{H} = \sum_{i=1}^{2} \left[\frac{p_i^2}{2m} + \frac{\kappa}{2}\, x_i^2 \right] + \frac{\kappa}{2}\, (x_2 - x_1)^2,$$

is invariant under the operation of *inversion*. That is, an inversion of the system through the mid-plane, which takes $x_1 \mapsto -x_2$ and $x_2 \mapsto -x_1$, leaves the Hamiltonian invariant.

A lengthy normal mode analysis shows that the energy eigenvectors are

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

This means there are two distinct modes of vibration, one in which the masses move in opposite directions and by equal amounts and one in which the masses move in the same direction and by equal amounts.

We can exploit the symmetry of this problem to obtain the same result, but with much less effort. Let I be the inversion operator. Since the Hamiltonian is invariant under the inversion operation, I commutes with H and thus the eigenvectors of I are also the eigenvectors of H. Writing the displacements x_1 and x_2 as the components of a vector $\mathbf{u}$ we have

$$I\mathbf{u} = I \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -x_2 \\ -x_1 \end{pmatrix}. \tag{1.1}$$

If the vector $\mathbf{u}$ is an eigenvector of I then we have

$$I\mathbf{u} = \begin{pmatrix} -x_2 \\ -x_1 \end{pmatrix} = \lambda\, \mathbf{u}, \tag{1.2}$$

where λ is the eigenvalue, and applying the inversion operation once more we obtain

$$\begin{aligned} I^2\mathbf{u} &= \lambda^2\mathbf{u} \\ &= I(I\mathbf{u}) = I \begin{pmatrix} -x_2 \\ -x_1 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \mathbf{u}. \end{aligned} \tag{1.3}$$

Thus $\lambda^2 = 1$, and the eigenvalues of I are $\lambda = \pm 1$, with corresponding eigenvectors

$$\mathbf{u}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \mathbf{u}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{1.4}$$

which are identical to those of the Hamiltonian. They describe the displacement amplitudes of the masses during normal mode vibrations and are either even or odd with respect to the inversion symmetry.

We learn that for a classical system with a symmetric one-dimensional potential $V(x)$, the eigenfunctions are of either odd or even parity, and we have seen how this knowledge can be used to simplify finding the solution to a problem. Quantum systems are generally much more complicated. Except for a few important but relatively simple systems, such as the hydrogen atom, the harmonic oscillator, and the Kronig–Penney model for a periodic lattice, most problems in quantum mechanics must be solved numerically.

Because the calculations are often long and tedious, and much effort is devoted to numerical methods, accuracy becomes a concern. Fortunately, some simplifications based on *symmetry* can be *rigorously* made. These usually involve the construction of *symmetry projection operators*, which are, in turn, based on the concept of *irreducible representations* (Irreps) and their characters. We will develop the ideas of *characters* and *representations* in Chapters 3–5. Here we state only that they play an all-important role in group theory.

We will present in Chapters 5 and 7 exact computational procedures for the calculation of matrix Irreps and characters using a method proposed by John Dixon in 1967. However, we stress here only that all the important quantitative symmetry information can be obtained with the aid of simple computer calculations.

1.2 Hamiltonians, eigenfunctions, and eigenvalues

A typical problem in condensed matter physics involves the determination of the physical states of a system given its Hamiltonian or its free energy. Consequently, the symmetry we need to exploit is, generally, that of the Hamiltonian. The application of symmetry will then require the definition of the corresponding operators and the specification of the rules of the action of these operations. Since a Hamiltonian can be defined on the configuration space of the physical system, we define a symmetry operation as a transformation effected on this configuration space. An example is the inversion operator I, which effects a vector transformation

$$\mathbf{r} \mapsto -\mathbf{r}.$$

Other typical operations are reflections, rotations, and translations. We write the transformation involving a symmetry operator $\hat{O}$ as

$$\hat{O}\,\mathcal{H}\,\hat{O}.$$

We start by collecting the symmetry operations that leave the Hamiltonian $\mathcal{H}$ *invariant*, i.e. those whose action leaves $\mathcal{H}$ unchanged. We designate this set of operations the *symmetry group*[1] of $\mathcal{H}$. If $\hat{O}$ is such an operator, then

$$\hat{O}\,\mathcal{H}\,\hat{O}^{\dagger} = \mathcal{H} \tag{1.5}$$

or

$$\hat{O}\,\mathcal{H} = \mathcal{H}\,\hat{O}. \tag{1.6}$$

Thus, if $\hat{O}$ leaves the Hamiltonian invariant, it must commute with the Hamiltonian. But what is the effect on an eigenfunction belonging to $\mathcal{H}$? We have

$$\mathcal{H}\,\Psi_i = E_i\,\Psi_i \tag{1.7}$$

[1] The word group will be justified in Chapter 2.

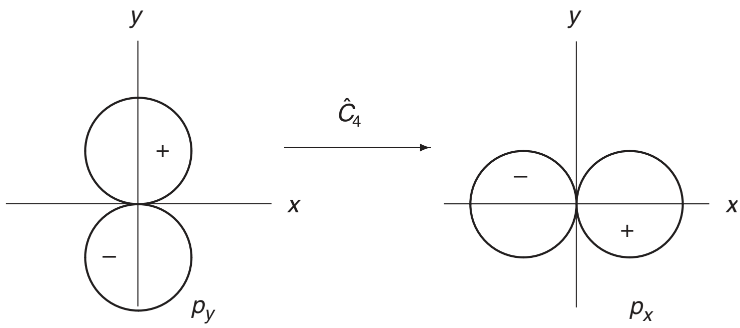

Fig. 1.6. $\hat{C}_4$ acting on p_y produces p_x.

which, when operated on by $\hat{O}$, gives

$$\hat{O}\,(\mathcal{H}\,\Psi_i) = \hat{O}\,(E_i\,\Psi_i). \tag{1.8}$$

Since the symmetry operator $\hat{O}$ commutes with $\mathcal{H}$, as described by (1.6), we obtain

$$\mathcal{H}\,(\hat{O}\,\Psi_i) = E_i\,(\hat{O}\,\Psi_i), \tag{1.9}$$

and we see that if Ψ_i is an eigenfunction, $\hat{O}\Psi_i$ is also an eigenfunction of the same Hamiltonian with the same eigenvalue E_i.

From quantum mechanics it is known that two commuting operators share a common set of eigenfunctions. Here we learn that by operating on an eigenfunction with a symmetry operator we generate another eigenfunction belonging to the same eigenvalue.

A pictorial example of the generation of a new eigenfunction with a symmetry operator is shown in Figure 1.6, it depicts the generation of a p_x-orbital by operating on a p_y-orbital with a $\pi/4$ rotation about the z-axis.

This example illustrates that the symmetry operators also act on functions defined on configuration space.[2]

All functions generated by the successive application of the operator $\hat{O}$ and all other symmetry operators of the system form a degenerate manifold in the Hilbert space of the Hamiltonian. The family of functions forming the basis of this manifold is classified by some characteristic symmetry properties, which distinguish it from other classes or families of functions in the Hilbert space.

To illustrate this property of generating distinct families of functions in Hilbert space, we consider the consequence of space isotropy, which is encountered under many guises

[2] A note on *function-space operators*
Function-space operators are generally denoted by a "hat" over the symbol for the operator, as in $\hat{O}$. This is not formally necessary in that it is possible to infer the nature of the operator by its context. If an operator acts on a function it is a function operator. Thus, sometimes, to reduce clutter, it may be convenient to not use a hat. Indeed, we do not use a hat over the Hamiltonian, which operates on wavefunctions. However, prudent practice is to use the hat for emphasis, since there are subtle differences in the action of a function operator on the coordinate variables of a function and the action of a configuration-space operator on the coordinates of a physical entity. This will be made clear in later sections of this chapter.

in mechanics, electromagnetics, and quantum mechanics. It is manifest in the family of functions we know as *spherical harmonics*, Y_l^m, which form disjoint subspaces denoted by the index l, each subspace l has dimension $2l+1$.[3]

Since isotropy means invariance under arbitrary infinitesimal rotations, it implies that a system with such symmetry should be invariant under all possible rotation operations. In quantum mechanics, isotropic symmetry of a system implies that all such operations should commute with its Hamiltonian, and thus their application to the eigenfunctions of the Hamiltonian should reveal the degeneracy within each spherical harmonic manifold in its Hilbert space.

In classical mechanics and electromagnetics, as well as in quantum mechanics, the closure of the different manifolds is demonstrated by the well-known *addition theorem* of Legendre polynomials. In essence these relations express the fact that pure angular rotations of, for example, p-states about their origin result in another p-state and thus do not alter the angular characteristics of the eigenfunction. Similar rotations of a dipole produce only other dipoles, not other multipoles.

The existence of a set of classes of symmetries to which symmetrized functions distinctly belong in isotropic space, that is, the *spherical harmonics*, is not an isolated case. It is the general feature for any underlying configurational symmetry. For example, the homogeneity of space leads to the natural adaptation of *plane-wave* functions as a distinct set for classifying symmetrized functions in this configuration space. The symmetry classes associated with a given symmetry group are conventionally known as its *irreducible representations*.

Another example may be found in quantum systems for which the symmetry of indistinguishability among a set of particles leads to two distinct and disjoint classes of wavefunctions which are commonly referred to as fermion and boson wavefunctions, or particle systems. To underscore the connection between the symmetry and the nature of the allowed states of such systems let us review the argument behind this well-established classification. The indistinguishability of the particles requires that the associated Hamiltonian should not change when two particles are exchanged, that is, $\mathcal{H}$ is invariant under such an exchange, or *permutation*, operation. If we denote the operator associated with a two-particle permutation operation by $\hat{P}_{12}$, we may write

$$\hat{P}_{12}\,\mathcal{H}\,\Psi = \mathcal{H}\,\hat{P}_{12}\,\Psi = E\,\hat{P}_{12}\,\Psi. \tag{1.10}$$

Now, the commutation of $\hat{P}_{12}$ with $\mathcal{H}$ requires that they share common eigenfunctions. If we consider the eigenfunctions of $\hat{P}_{12}$, we have

$$\hat{P}_{12}\,\Psi = \lambda\,\Psi, \tag{1.11}$$

which means the exchange operation leaves the state unchanged apart from a multiplicative, possibly complex, factor λ. A second application of $\hat{P}_{12}$ returns the system to its original configuration, so that

$$\hat{P}_{12}^{\,2}\,\Psi = \lambda^2\,\Psi = \Psi, \tag{1.12}$$

[3] In electromagnetics the spherical harmonics describe monopole, dipole, quadrupole, … fields, and in atomic physics they are manifest as $s, p, d, \ldots$ states. Indeed, the structure of the periodic table of the elements is a consequence of the three-dimensional isotropic character of space.

hence

$$\lambda^2 = 1 \tag{1.13}$$

or $\lambda = \pm 1$, thus establishing *two distinct classes of eigenstates* of a Hamiltonian describing a set of indistinguishable particles, namely, those that transform even and those that transform odd under the permutation or particle-exchange operation.

1.2.1 Examples of symmetry and conservation laws

Translation and conservation of linear momentum

Given a classical system's Hamiltonian $\mathcal{H}(x, p)$, where x and p are conjugate coordinate and momentum variables, we write the canonical equations of motion as

$$\dot{x} = \frac{\partial \mathcal{H}}{\partial p},$$
$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial x}.$$

If the system is invariant under arbitrary translations, then the r.h.s of the second equation vanishes and the linear momentum p is conserved. When the system is treated quantum mechanically, we define the translation operator corresponding to an infinitesimal displacement dx as

$$R(dx)\, x = x + dx,$$

and, as we will show in Section 1.3, its action on function-space is given by

$$\hat{R} \mid \psi(x) \rangle = \mid \psi(x - dx) \rangle = \mid \psi(x) \rangle - i\frac{p}{\hbar} dx \mid \psi(x) \rangle,$$

so that the operator $\hat{R}$ can be expressed as

$$\hat{R} = \exp\left(-i\,\frac{p\,dx}{\hbar}\right). \tag{1.14}$$

If the Hamiltonian is invariant under such operations, then

$$[\,\hat{R}, \mathcal{H}\,] = 0. \tag{1.15}$$

Using Heisenberg's equation of motion and substituting (1.14), we obtain

$$\frac{d}{dt}\langle p \rangle = \frac{1}{i\hbar}\,\langle [\,p, \mathcal{H}\,] \rangle = 0. \tag{1.16}$$

Inversion and parity conservation

Consider a system which remains invariant under the inversion operation, i.e.

$$[\,\hat{I}, \mathcal{H}\,] = 0, \tag{1.17}$$

then we find that it also commutes with the time-translation operator

$$\hat{U}(t_2, t_1) = \exp\left[-i\frac{\mathcal{H}\,(t_2 - t_1)}{\hbar}\right] \;\Rightarrow\; [\,\hat{I}, \hat{U}\,] = 0.$$

Since $\hat{I}$ commutes with $\mathcal{H}$, they have simultaneous eigenfunctions, such that

$$\hat{I} \,|\, \psi(t_1)\,\rangle = \lambda_1 \,|\, \psi(t_1)\,\rangle. \tag{1.18}$$

Since $\hat{I}^2$ is the identity, λ_1 assumes the values ± 1 only, and we obtain

$$\begin{aligned} \hat{I} \,|\, \psi(t_2)\,\rangle &= \hat{I}\,\hat{U}(t_2, t_1) \,|\, \psi(t_1)\,\rangle = \hat{U}(t_2, t_1)\hat{I} \,|\, \psi(t_1)\,\rangle \\ &= \lambda_1 \hat{U}(t_2, t_1) \,|\, \psi(t_1)\,\rangle = \lambda_1 \,|\, \psi(t_2)\,\rangle\,. \end{aligned} \tag{1.19}$$

1.3 Symmetry operators and operator algebra

We introduced earlier the idea that symmetry operators may act on Hamiltonians as well as functions, and that these actions can be regarded as transformations in configuration space. Here, we shall give a detailed exposé of these ideas, and establish some concepts and conventions needed in order to be self-consistent in applying symmetry operations to physical applications of group theory.

1.3.1 Configuration-space operators

Configuration space is the real physical space in which physical objects move, i.e. where we define classical particle trajectories and quantum mechanical wavefunctions and probabilities. Operators acting in this space are known as *configuration-space operators*. Now, we consider a point object P, a particle in this space, located at position $\mathbf{r}$ with respect to the reference axes, as shown in Figure 1.7. If the object is translated by a vector $\mathbf{t}$, it will arrive at the new position defined by the vector $\mathbf{r}'$ with respect to the axes such that

$$\mathbf{r}' = \mathbf{r} + \mathbf{t}. \tag{1.20}$$

We can thus define an *active operator* t_A, and its inverse t_A^{-1} such that

$$\begin{aligned} t_A\mathbf{r} &= \mathbf{r} + \mathbf{t} \\ t_A^{-1}\mathbf{r} &= \mathbf{r} - \mathbf{t}. \end{aligned} \tag{1.21}$$

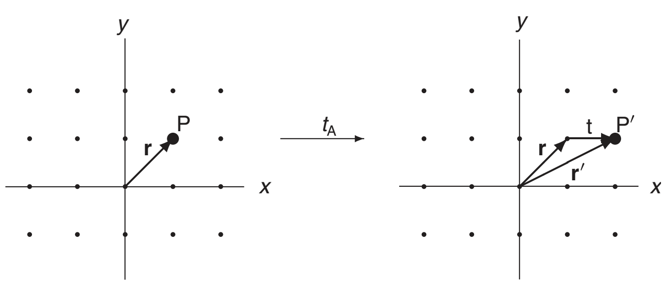

Fig. 1.7. Active operator t_A translates the point body P from $\mathbf{r}$ to $\mathbf{r}'$.

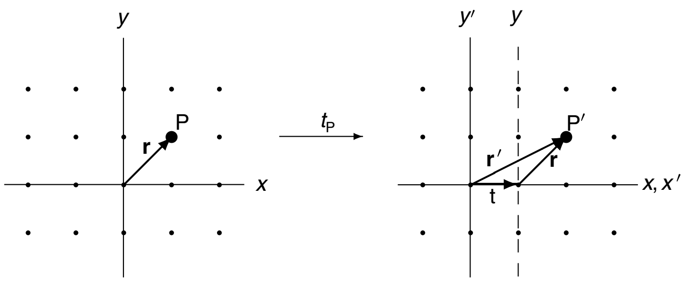

Fig. 1.8. Passive operator t_{P} translates the coordinate system by $-\mathbf{t}$.

We show a grid of equivalent points in configuration space because we have in mind, say, a crystal structure in which all the grid points correspond to atomic positions. In such a case, moving one point (atom) P of a body (a crystal) moves *all* the points. The space is infinite, as is the (idealized) crystal. In Figure 1.7, we show the identical fixed coordinate system twice in order to see the before and after pictures.

Now consider instead the effect of the *passive operator*, t_{P}, which translates the coordinate axes by $-\mathbf{t}$ while keeping the point object fixed, as in Figure 1.8. Then the new position of the point P after the translation is still given by

$$t_{\mathrm{P}}\mathbf{r} = \mathbf{r}' = \mathbf{r} + \mathbf{t}, \tag{1.22}$$

but the interpretation is different. The new position is with reference to the new x', y' coordinate system. The operator t_{P} has the inverse effect from that of t_{A}.

Likewise, rotation operations can be either passive or active, bearing inverse relations to each other.

1.3.2 Function-space operations

We have alluded to a connection between configuration-space operators and function-space operators. As a prelude to showing that a coordinate transformation in configuration space *induces* a transformation of the function defined on it, we consider the case of a traveling wave. This contains the basic physics and mathematics in a familiar and easily understood situation.

Consider a transverse wave of shape $f(x,t)$ traveling with positive velocity along the x-axis, as shown in Figure 1.9. If we are to deal with the wave motion quantitatively, we need a mathematical description of the shape of the wave moving as a whole. We assume no damping or dispersion, so the shape remains unchanged, and any point on the wave may be taken as a reference point. We will follow the motion of the wave peak. To describe an amplitude that remains constant, although its position moves to the right with increasing time, we need a function of the general form

$$f(x,t) = f(x - vt). \tag{1.23}$$

With a function of this form, as t increases, x also increases, but the increase in x is exactly compensated for in the argument of f by the term $-vt$, so that the argument is