Unless noted otherwise, the Einstein summation convention is used: repeated indicies of vectors and tensors are summed, e.g., \( \mathbf{A} \cdot \mathbf{B} = \sum_{i=1}^{3} A_i B_i \equiv A_i B_i \).

1. Generalized Lagrangian Classical Mechanics

Classical mechanics can be formulated with a variational principle and the calculus of variations, as an alternative to the simple Newtonian form:

\[
m\ddot{x}_i = F_i = -\frac{\partial V}{\partial x},
\]

where \( x_i \) is the Cartesian coordinate of a point particle of mass \( m \), \( F_i \) is the external force applied to the particle, and the force is assumed to be conservative, the negative gradient of a potential energy function \( V(x) \). Newtonian mechanics for rigid bodies can be formulated in a similar way, and this approach can even be extended to relativistic point mechanics.

The calculus of variations uses functionals, functions of functions, \( F[f] \). In a functional, the independent “variable” is a whole function; the functional \( F \) maps a given function to a number: \( F[f] : f \rightarrow F \). Typically, the \( F[f] \) is constructed as an integral over an integrand involving some function \( f \). The calculus of such functionals varies the independent function \( f \) to see what happens to the functional value \( F \). The variations are denoted by \( \delta : f \rightarrow f + \delta f \) maps to \( F \rightarrow F + \delta F \).

In classical mechanics, the path in space \( x_i(t) \) is the independent function. The key functional is the action \( S[x, \dot{x}] \):

\[
S = \int_{t_i}^{t_f} dt \ L(x, \dot{x}) , \quad L = \frac{1}{2} m \dot{x}^2 - V(x) ,
\]

where \( L(x, \dot{x}) \) is the Lagrangian function for the particle. The initial and final times \( t_i \) and \( t_f \) are fixed. The path the particle takes is that path minimizing (extremizing) the action \( S \):

\[
\delta S = \int_{t_i}^{t_f} dt \left[ m \ddot{x} \cdot \delta \dot{x} - \frac{\partial V}{\partial x} \delta \dot{x} \right] = \int_{t_i}^{t_f} dt \left[ -m \dddot{x} - \frac{\partial V}{\partial x} \right] \delta x + \left[ m \ddot{x} \cdot \delta x \right]_{t_i}^{t_f} = 0 ,
\]

where integration by parts has been applied in the second line. If there are no constraints, each coordinate is independent, and, if the endpoint initial and final conditions are held fixed, the last term vanishes. Newton’s equations then follow for each of the three Cartesian coordinates. This variational form is Hamilton’s principle, although this form was first stated by Lagrange (1788). The Lagrangian \( L \) and action \( S \) can be extended to multiparticle and rigid body systems.

The nice thing about this generalized or Lagrangian mechanics is that the variational method can be applied no matter how we choose to represent the coordinates. So we can transform the Cartesian \( x_i \) to some other set of generalized coordinates \( q_a = q_a(x; t) \). The function \( L \) and the functional \( S \) are scalars and so don’t care what coordinates we use, as long as the transformation from \( x \) to \( q \) is unique, invertible, and non-singular. We can
rewrite $L$ and $S$ as function and functional, respectively, in terms of the $q_a$ and derive the same set of Euler-Lagrange equations of motion:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_a}\right) - \frac{\partial L}{\partial q_a} = 0$$  \hspace{1cm} (4)

for each independent coordinate $q_a$. The same formal equations are valid for these new, non-Cartesian and possibly even non-inertial, coordinates. The term $p_a = \partial L/\partial \dot{q}_a$ is the generalized momentum for $q_a$, and the second term in (4) is (negative) the generalized force $F_a$. Thus $\dot{p}_a = F_a$.

Constraints, with redundant (extra) coordinates, can be added into the action using Lagrange multipliers. Each extra term added to $L$ has the form $\lambda_r G_r(q, \dot{q}; t)$, where the corresponding constraint is $G_r(q, \dot{q}; t) = 0$ and $\lambda_r$ is the Lagrange multiplier for the $r$th constraint.

The variational approach to obtaining dynamical equations has a distinguished history beginning with Euler and Lagrange and has been applied, starting with Hamilton’s work on ray optics, to every branch of mathematical physics.

2. Hamiltonian Form of Classical Mechanics

The Lagrangian form of generalized mechanics uses the $q, \dot{q}$ as independent coordinates and velocities. Since the dynamics is determined only by the second derivatives of the $q$, we need to treat the zeroth and first derivatives as independent pieces of information about the system.

Recall $p_a = \partial L/\partial \dot{q}_a$ is the generalized momentum. We could use, in place of the $\dot{q}$, the $p$, so that the state of the mechanical system is specified by pairs of $(q, p)$ instead. The master function in that case is the Hamiltonian $H(q, p) = p_a \dot{q}_a - L$, where the $\dot{q}$ must be eliminated in favor of the $p$. Then $H$ is a function of the $(q, p)$, not the $(q, \dot{q})$. The relationship of $H$ to $L$, with the replacement of one independent variable $\dot{q}$ by another $p$, is a type of Legendre transformation. Hamilton’s principle now takes on Hamilton’s own form (1827):

$$\delta S = \int dt \delta[p_a \dot{q}_a - H] = 0 \hspace{1cm} ,$$

$$\dot{q}_a = \frac{\partial H}{\partial p_a} \hspace{1cm} , \hspace{1cm} \dot{p}_a = -\frac{\partial H}{\partial q_a} \hspace{1cm} .$$  \hspace{1cm} (5)

The variations of $q_a$ and $p_a$ are taken to be independent. These equations are first-order in time, two equivalent ones for every one of the second-order Euler-Lagrange equations. Under some general restrictions, $H = E =$ the total energy of the system.

The state of a mechanical system at an instant of time $t$ is specified by all of the $q_a(t), p_a(t)$. If there are $N$ coordinates, the $2N$-dimensional space of all $(q, p)$ is the system’s phase space. The instantaneous state is a point in phase space. If the state at any time is unique, its subsequent evolution is also unique. Thus different paths in phase space are unique, never branching or merging. Furthermore, through any point in phase space passes one and only one time evolution path. System information in phase space is conserved.

This conservation of information has important consequences in statistical mechanics, the foundation of thermodynamics. In a statistical treatment, one does not know the system’s initial conditions, but rather an initial region of phase space. The information-conservation property implies that the phase space volume occupied by the system does not change as the system evolves, though we do not know the unique path the system takes. In equilibrium thermodynamics, this is equivalent to the system’s entropy remaining constant. The entropy is essentially the logarithm of the occupied phase space. A system’s entropy can change, but only if heat is added or the system’s boundaries are changed. In that
case, the system is no longer isolated and the information-conservation property no longer holds.

3. Classical Mechanics and Group Theory

The action form of classical mechanics facilitates the introduction of group theory. A symmetry of the mechanical system is said to be “good” if the corresponding group operation, acting on the coordinates and/or velocities and/or the time, leaves the action unchanged. This has an important consequence for continuous groups and symmetries.

Consider transforming the $q_a$ by a group operation: $q'_a = G(q_a)$. If $G$ is continuous, let there be an infinitesimal form, $q'_a = q_a + \epsilon G_{ab} q_b$, with $\epsilon \ll 1$. (Other forms of infinitesimal transformation can also be constructed.) If the $G_{ab}$ are all independent, they are called the generators of the group operation, written in a particular representation to act on the generalized coordinate set $q_a$. I assume the $G_{ab}$ to be time-independent. Applying the infinitesimal form of $G$ to $S$, we get for the shift of $S$

$$\delta S = \int_{t_i}^{t_f} dt \left[ \frac{\partial L}{\partial q_a} \delta q_a + \frac{\partial L}{\partial \dot{q}_a} \delta \dot{q}_a \right] = \int_{t_i}^{t_f} dt \; \epsilon G_{ab} \left[ \frac{\partial L}{\partial q_b} q_a + \frac{\partial L}{\partial \dot{q}_b} \dot{q}_a \right]$$

(6)

where the last line is obtained using the Euler-Lagrange equations. If each $G_{ab}$ is independent, then the quantities $Q_{ab}$ are conserved (constants of the motion):

$$\frac{dQ_{ab}}{dt} = d \left( \frac{\partial L}{\partial \dot{q}_a} q_b \right) = 0 \; .$$

(7)

This result, which can be generalized to other types of continuous transformations, also has a converse: any conserved quantity can be related to the generator of a continuous symmetry group of the system. The general theorem was first proved by Emmy Noether (1918): to each independent generator of a good continuous symmetry transformation in a physical system corresponds a conserved quantity, and vice versa.

The symmetry-conservation law relationship is helpful in classical mechanics for identifying constants of the motion. These in turn are essential for reducing the complexity of the mechanical equations during integration. In special cases with a high level of symmetry, exact (analytic) solutions to the Lagrangian equations of motion can be found using the conserved quantities. As the system evolves in time $q_a(t)$, the quantities $Q_{ab}(t) = Q_{ab}(0)$ remain constant and determined solely by the initial conditions and the symmetry of the system. Distinct solutions of the equations of motion can be labelled uniquely by different values of the $Q_{ab}$.

The most basic symmetries of any physical system are its spacetime symmetries. The physics of an isolated system is unchanged if it is (i) translated in space by a fixed amount; (ii) rotated in space by a fixed angle about a fixed axis; (iii) translated in time by a fixed amount; and (iv) boosted from an old to a new inertial frame. Each of these symmetries has a corresponding conserved quantity: total linear momentum $P$ of the system (space translation); total angular momentum $L$ of the system (space rotation); total energy $E$ of the system (time translation); and mass $m$ of particle (boost).
Unless noted otherwise, the Einstein summation convention is used: repeated indicies of vectors and tensors are summed, e.g., \( \mathbf{A} \cdot \mathbf{B} = \sum_i A_i B_i \equiv A_B \).

1. Further Notes on Hamiltonian Classical Mechanics — Poisson Brackets

The master function for classical mechanics is the Lagrangian \( L \), a function of generalized coordinates \( q^a \) and velocities \( \dot{q}^a \). \( L = T - V \), where \( T \) is the kinetic and \( V \) the potential energy. The \((q^a, \dot{q}^a)\) in turn are functions of the independent time variable \( t \). The action functional \( S \) is constructed from \( L \):

\[
S = \int_{t_i}^{t_f} dt \ L(q, \dot{q}) \quad , \quad L = T(q, \dot{q}) - V(q) \quad ,
\]

where the initial and final times \( t_i \) and \( t_f \) are fixed. The path the particle takes is that path minimizing (extremizing) the action \( S \):

\[
\delta S = 0 \quad , \quad \delta S = 0,
\]

are the Euler-Lagrange equations. Each equation is second-order in time. Constraints can be added to \( L \) using Lagrange multipliers. Letting \( p^a = \partial L / \partial \dot{q}^a \) be the generalized momentum conjugate to \( q^a \) and \( F^a = \partial L / \partial q^a \) be the generalized force along the “\( a \)” direction, we have a generalized Newton’s second law for each \( q^a \).

The equivalent Hamiltonian form starts with the Legendre transformation from \( L(q, \dot{q}) \) to \( H(q, p) \):

\[
H(q, p) = p^a \dot{q}^a - L(q, \dot{q}) \quad , \quad S = \int_{t_i}^{t_f} dt \ [p^a \dot{q}^a - H] \quad .
\]

We have to solve \( p^a = p^a(q, \dot{q}) \) to express \( \dot{q}^a = \dot{q}^a(q, p) \), then rewrite \( S \) as a functional of \((q, p)\). The Hamiltonian variational principle extremizes \( S \) with respect to variations in \((q, p)\), treating \( q \) and \( p \) as independent. Instead of one second-order equation for each \( q^a \), we get two first-order equations, one for \( q^a \) and one for \( p^a \):

\[
\delta S = \int dt \ \delta [p^a \dot{q}^a - H] = 0 \quad ,
\]

\[
\dot{q}^a = \frac{\partial H}{\partial p^a} \quad , \quad \dot{p}^a = -\frac{\partial H}{\partial q^a} \quad .
\]

The space of all \((q^a, p^a)\) is phase space \( \Pi \). A point in \( \Pi \) specifies the state of the system uniquely. Under certain broad conditions, \( H = E = \) total energy of the system.

Any real physical observable \( A \) that we wish to measure in this system must then be a function on \( \Pi \) and expressible as a function of the \((q^a, p^a)\) and perhaps also explicitly of time \( t \) : \( A = A(q, p; t) \). Then

\[
\frac{dA}{dt} = \frac{\partial A}{\partial q^a} \frac{dq^a}{dt} + \frac{\partial A}{\partial p^a} \frac{dp^a}{dt} + \frac{\partial A}{\partial t} = \frac{\partial A}{\partial q^a} \frac{\partial H}{\partial p^a} - \frac{\partial A}{\partial p^a} \frac{\partial H}{\partial q^a} + \frac{\partial A}{dt} \quad .
\]
This form inspired Poisson brackets (Poisson around 1820, then Hamilton around 1830). Let \( A(q, p; t) \) and \( B(q, p; t) \) be two physical observables. Then the Poisson bracket \( \{ A, B \} \) is
\[
\{ A, B \} \equiv \frac{\partial A}{\partial q_a} \frac{\partial B}{\partial p_a} - \frac{\partial B}{\partial q_a} \frac{\partial A}{\partial p_a} .
\] (6)

Thus
\[
\frac{dA}{dt} = \{ A, H \} + \frac{\partial A}{\partial t} .
\] (7)

A conserved quantity \( Q \) does not change as the system evolves. Any \( Q \) is a generalized observable: \( Q = Q(q, p) \), and \( \dot{Q} = 0 \) yields \( \{ Q, H \} = 0 \). If the conservation of \( Q \) is associated with a continuous symmetry of the system, Noether’s theorem implies each conserved \( Q \) is proportional to each group generator that leaves the system unchanged (invariant) under the symmetry group transformation.

2. Hamiltonian Quantum Mechanics

The entire need for quantum mechanics arises from one universal physical constant, Planck’s constant \( h \) (Planck, 1900). In ordinary units, this number is very small: \( h = 6.63 \times 10^{-34} \) Joule-sec. In everyday situations, the smallness of \( h \) makes quantum mechanics invisible. The units of \( h = \text{energy} \times \text{time} \) suggest a connection with the action \( S \), which carries the same units. A system’s underlying quantum dynamics is indistinguishable from classical mechanics if the action \( S(i \rightarrow f) \) going from the initial \( i \) to the final state \( f \) is large: \( S(i \rightarrow f) \gg h \). But if \( S(i \rightarrow f) \) is comparable to \( h \), the system must be described using quantum mechanics. This is always true for isolated microscopic systems (atoms, molecules, nuclei, elementary particles), as well as for certain macroscopic systems such as superconductors and superfluids.

Assume we have a system with \( q \)'s and \( p \)'s, and a Hamiltonian function \( H(q, p) \). To translate the system’s dynamics from classical to quantum form, or “quantize” it, we need some quantum axioms (Dirac, 1930; von Neumann, 1932).

**Axiom # 1** The physical state of any system is completely described by a time-dependent state vector \( |\psi(t)\rangle \). The state vector lives in a complex Hilbert space \( \mathcal{H} \) that encompasses all possible states of the system.

**Axiom # 2** To each real classical physical observable \( A(q, p) \), starting with the \( q \)'s, the \( p \)'s, and \( H(q, p) \) itself, corresponds a Hermitian or self-adjoint operator \( \hat{A} \) acting on this Hilbert space. The space \( \mathcal{H} \) is self-dual and contains the conjugate state vector \( \langle \psi | = (|\psi\rangle)^\dagger \) as well.

If we think of a particular representation of vectors and operators, any vector in \( \mathcal{H} \) is a complex column vector and its conjugate as the conjugated row vector. The Dirac notation is used here: vectors are “kets” \( |\psi\rangle \), while their conjugates \( \langle \psi | \) are “bras”. Hence the inner product of two vectors is \( \langle \phi | \psi \rangle \), a “bra-ket” or “bracket”. The complex conjugate of an inner product is \( \langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle \).

The Hamiltonian operator \( \hat{H} \) generates the system’s time evolution.

**Axiom # 3** The state vector evolves in time via the time-dependent Schroedinger equation:
\[
i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle ,
\] (8a)

where the reduced Planck’s constant \( \hbar = h/2\pi \). The formal solution is:
\[
|\psi(t)\rangle = \exp(-i\hat{H}t/\hbar)\psi(0)\rangle .
\] (8b)
The exponential of an operator is defined by its power series. Already, group theory has silently crept in: time $t$ forms a one-dimension manifold upon which $\hat{H}$ generates the evolution of the state vector as a group translation. That is, $\hat{H}$ generates time translations, echoing the classical Noether theorem: time translation invariance generates a conserved energy $E = H$.

3. The Classical-Quantum Correspondence

The state vector cannot be measured directly. Instead classical observables $A(q, p; t)$ are measured. In a classical system, the resulting value of $A$ is unambiguous, since the values of $q_a(t)$, $p_a(t)$, and $t$ are known. Not so in quantum mechanics.

**Axiom # 4** The possible values resulting from a measurement of a real classical observable $A(q, p; t)$ in a quantum system are given by the spectrum of eigenvalues $\{a_i\}$ of the corresponding quantum operator $\hat{A}$.

Since $\hat{A}$ is Hermitian, its eigenvalues $\{a_i\}$ are real and the corresponding eigenvectors $|a_i\rangle$ are orthogonal: $\langle a_i | a_j \rangle = 0$ if $i \neq j$. The eigenvectors can be normalized to one, such that $\langle a_i | a_i \rangle = 1$. (For a continuous spectrum, replace $\delta_{ij}$ by the Dirac delta function.)

If a measurement of $A$ is made, one of the $\{a_i\}$ will result. Which one cannot be predicted. Quantum mechanics is deterministic in the sense that given an initial state $|\psi(0)\rangle$, the later state $|\psi(t)\rangle$ can be generated uniquely. But if we now ask for the values of classical observables $A$, quantum mechanics cannot predict these uniquely. Instead it predicts something weaker, the probabilities of getting some eigenvalue $a_i$ from measuring $A$.

**Axiom # 5** The probability $P(a_i; t)$ that a particular eigenvalue $a_i$ will result from a measurement of $A$ is given by the norm-square of the projection of $|\psi(t)\rangle$ on to $|a_i\rangle$.

$$P(a_i; t) = |\langle a_i | \psi(t) \rangle|^2 . \tag{9}$$

Upon measurement at time $t_m$, the Schrödinger evolution of $|\psi(t)\rangle$ is instantaneously interrupted; the system is “reinitialized” to the corresponding eigenvector, then subsequently evolves normally: $|\psi(t_m)\rangle = |a_i\rangle$.

The state vector can be decomposed by projection on to a complete set of basis vectors $|i\rangle$. The eigenvectors of a Hermitian $\hat{A}$ form such a basis. Thus decompose the identity operator into projection operators over the orthonormal basis $|a_i\rangle$:

$$\hat{1} = \sum_i |a_i\rangle \langle a_i| , \quad |\psi(t)\rangle = \sum_i \langle a_i | \psi(t) \rangle |a_i\rangle . \tag{10}$$

The respective probabilities of $A$ taking on a particular eigenvalue $a_i$ at a time $t$ are given by the norm-squared components of the state vector in the eigenbasis $\{|a_i\rangle\}$.

Since projection of $|\psi(t)\rangle$ on to eigenvectors generates probabilities, the sum over all possibilities spans the space and exhausts all possible physical states of the system. Thus

$$\langle \psi(t) | \psi(t) \rangle = 1 , \quad \text{for all time } t .$$

This normalization condition is preserved by the time evolution (8). The conservation of probability or unitarity is the quantum analog to conservation of volume in classical phase space $\Pi$.

The indeterminacy of classical observables $A$ becomes clear if a few, isolated measurements of identical systems are made. Measurements will not yield the same value $A(q, p; t)$
over and over. Instead the spectrum of eigenvalues \( \{a_i\} \) appears, with a probability distribution given by (9). But a correspondence can still be made to classical notions if we define an expectation value of \( \hat{A} \), \( \langle A \rangle \equiv \langle \psi(t)|\hat{A}|\psi(t) \rangle \). Expand \( |\psi(t)\rangle \) in the eigenbasis \( \{|a_i\rangle\} \).

\[
\langle A \rangle = \langle \psi(t)|\hat{A}|\psi(t) \rangle = \sum_i \sum_j \langle \psi(t)|a_j\rangle \langle a_j|\hat{A}|a_i\rangle \langle a_i|\psi(t) \rangle \\
= \sum_i \sum_j \langle \psi(t)|a_j\rangle \langle a_j|a_i\rangle \langle a_i|\psi(t) \rangle \\
= \sum_i \sum_j \langle \psi(t)|a_j\rangle \cdot \delta_{ij} \cdot \langle a_i|\psi(t) \rangle \cdot a_i \\
= \sum_i \langle a_i|\psi(t) \rangle^2 \cdot a_i ,
\]

because \( \hat{A}|a_i\rangle = a_i|a_i\rangle \) and \( \langle a_j|a_i\rangle = \delta_{ij} \). That is, \( \langle A \rangle \) is a weighted average of its eigenvalues, each weighted by its respective probability \( P(a_i; t) \). Many repeated measurements of \( A \) in identical systems converge to \( \langle A \rangle \) in the statistical sense (Born, 1927).

Assume \( A \) contains explicit time dependence, in addition to the time dependence of the state \( |\psi(t)\rangle \). The expectation value evolves in time, in analogy to the classical case (5,7):

\[
\frac{d\langle A \rangle}{dt} = \frac{d}{dt} \langle \psi(t)|\hat{A}|\psi(t) \rangle \\
= \left( \frac{d}{dt} \langle \psi(t)| \right) \hat{A} |\psi(t) \rangle + \langle \psi(t)| \left( \frac{\partial}{\partial t} \hat{A} \right) |\psi(t) \rangle + \langle \psi(t)| \hat{A} \left( \frac{d}{dt} |\psi(t) \rangle \right) \\
= -\frac{1}{i\hbar} \langle \psi(t)|\hat{H}\hat{A}|\psi(t) \rangle + \langle \psi(t)| \left( \frac{\partial}{\partial t} \hat{A} \right) |\psi(t) \rangle + \frac{1}{i\hbar} \langle \psi(t)|\hat{A}\hat{H}|\psi(t) \rangle \\
= \langle [\hat{A}, \hat{H}] \rangle + \langle \frac{\partial A}{\partial t} \rangle .
\]

by using the original and conjugate of the Schroedinger equation (8). The commutator of two operators \( \hat{A} \) and \( \hat{B} \) is defined by \( [\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \). Comparing this to (7), the simplest way to make this result automatic is to make the commutators of quantum operators proportional to the Poisson brackets of the corresponding classical observables.

**Axiom # 6** The algebra of quantum operators is generated by the corresponding classical Poisson brackets:

\[
[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} = i\hbar \{A, B\} .
\]

The non-vanishing of \( \hbar \) necessitates the conversion of classical variables \( A \) and \( B \) into quantum operators \( \hat{A} \) and \( \hat{B} \) acting on \( \mathcal{H} \). In a discrete basis, the operators can be represented by non-commuting matrices. In a continuous basis, the operators are usually represented by non-commuting differential operators.

The most basic pair is \( x \) and \( p_x \) : \( \{x, p_x\} = 1 \), so \( [\hat{x}, \hat{p}_x] = i\hbar \). Since \( x \) is continuous, the differential representation is \( \hat{p}_x = -i\hbar (\partial / \partial x) \). That is, \( \hat{p}_x \) generates translations along the \( x \) direction. Analogously for \( \hat{p}_y \) and \( \hat{p}_z \) along \( y \) and \( z \) axes, respectively. Note the parallel to the classical Noether theorem for spatial translation symmetry: each invariance of a system along a particular direction in space implies conservation of the linear momentum \( \mathbf{P} \) component along that direction.
4. The Uncertainty Relation

The commutativity or lack thereof of any pair of Hermitian operators \( \hat{A}, \hat{B} \) leads to an important result about measurement in quantum systems.

If \([\hat{A}, \hat{B}] = 0\), the two operators can be simultaneously diagonalized in the space \( \mathcal{H} \). (The operators are diagonal in the eigenbasis, and the diagonal values are just the eigenvalues.) It is then possible to measure \( \hat{A} \) and get a definite eigenvalue \( a_i \), while simultaneously measuring \( \hat{B} \) and getting a definite eigenvalue \( b_j \). The consequence is that \( \hat{A} \) and \( \hat{B} \) can be measured simultaneously with infinite accuracy. Equivalently, the measurement of \( \hat{A} \) leaves the system in an eigenstate \( |a_i\rangle \) of \( \hat{A} \); but if \([\hat{A}, \hat{B}] = 0\), this state can also be an eigenstate \( |b_j\rangle \) of \( \hat{B} \).

If \([\hat{A}, \hat{B}] \neq 0\), however, the two operators cannot be simultaneously diagonalized. If \( \hat{A} \) is measured, leaving the system in an eigenstate \( |a_i\rangle \), the system cannot also be in an eigenstate \( |b_j\rangle \). And vice versa for \( \hat{B} \). The upshot is, \( \hat{A} \) and \( \hat{B} \) cannot be measured simultaneously with infinite accuracy. An eigenstate \( |a_i\rangle \) has non-zero inner product with multiple eigenvectors \( |b_j\rangle \) and multiple eigenvalues \( b_j \). And vice versa for \( |b_j\rangle \). A unique value for one is incompatible with a unique value for the other.

This limitation on simultaneous measurement of two observables can be made be quantitatively rigorous. From the expectation values \( \langle \hat{A} \rangle \) and \( \langle \hat{B} \rangle \), define variances of measurement:

\[
(\Delta A)^2 \equiv \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle, \quad (\Delta B)^2 \equiv \langle (\hat{B} - \langle \hat{B} \rangle)^2 \rangle.
\]  

(14)

The Schwarz inequality of linear algebra states \( \left| \langle \phi | \psi \rangle \right|^2 \leq \langle \phi | \phi \rangle \cdot \langle \psi | \psi \rangle \). (For real vectors, the inequality just means the cosine-squared of the angle between two vectors \( \leq 1 \).) This inequality can be used to prove the following result:

\[
\Delta A \cdot \Delta B \geq \left| \frac{[\hat{A}, \hat{B}]}{2} \right|.
\]  

(15)

Non-commutativity of two operators implies that the variances of their measurements cannot be simultaneously driven to zero by any possible experiment. The most famous version of (15) is the original result of Heisenberg (1927) for pairs of Cartesian coordinates and momenta:

\[
\Delta x \cdot \Delta p_x \geq \frac{\hbar}{2}, \quad \text{etc.}
\]  

(16)

The uncertainties of measuring \( x \) and \( p_x \) can only be “traded off” of one another. An actual experiment typically does much worse than (16), but such uncertainty relations place a lower bound on simultaneous measurement errors even in ideal experiments. The trade-off and non-commutativity are results of \( \hbar \neq 0 \).

The lack of determinacy for classical variables in the quantum world is intuitively captured by applying the Heisenberg relations (16) to \( \Pi \). Since position and momentum cannot be defined simultaneously, classical phase space is “fuzzed out”. An ideal quantum particle never occupies volume in \( \Pi \) less than \( \sim (\hbar/2)^3 \). Even if the quantum state \( |\psi(t)\rangle \) is unambiguous, the classical state cannot be defined more sharply than allowed by (16).
Unless noted otherwise, the Einstein summation convention is used: repeated indices of vectors and tensors are summed, e.g., $\mathbf{A} \cdot \mathbf{B} = \sum_{i=1}^{3} A_i B_i \equiv A_i B_i$.

### 1. Subspaces and Irreducible Group Representations

If $[\hat{A}, \hat{B}] = 0$, this pair can be measured simultaneously with infinite accuracy. The measurements result in some definite eigenvalues $a_i$ and $b_j$. But one operator, the Hamiltonian $\hat{H}$, is special, because it generates time evolution in quantum systems. Recall, if $\hat{A}$ has no explicit time dependence,

$$\frac{d\langle A \rangle}{dt} = \frac{\langle [\hat{A}, \hat{H}] \rangle}{i\hbar}. \quad (1)$$

If $\hat{A}$ commutes with the Hamiltonian $\hat{H}$, its expectation value does not change with time. The analogue in classical systems is a conserved quantity $A(q, p)$ whose Poisson’s bracket with $H(q, p)$ vanishes. But the quantum case is broader: In classical systems, conserved quantities map one-to-one with continuous symmetries (Noether’s theorem). Continuous symmetries also play this role in quantum systems, but quantum systems can also have “conserved” discrete labels for eigenstates associated with discrete symmetries. The next section presents an example of a discrete symmetry.

The quantum version of Noether’s theorem yields this fundamental result: if $A(q, p)$ is conserved as a consequence of a continuous symmetry group $G$ acting on a classical system, then $\hat{A}$ is a Hermitian generator of a representation of $G$ acting on the corresponding quantum system’s Hilbert space $\mathcal{H}$. The representation is important. Whatever the symmetry operation $G \in G$, when it acts on the classical system: $(q, p) \rightarrow (q', p')$, the particular representation of $G$ is obviously real. But when $G$ acts on the Hilbert space: $|\psi\rangle \rightarrow \hat{G}|\psi\rangle$, the group operator $\hat{G}$ must be in a complex, unitary representation: $\hat{G}^{-1} = \hat{G}^\dagger$, where $\hat{G}^\dagger$ is the Hermitian conjugate of $\hat{G}$. The Hilbert space is complex, and there is no reason to restrict $\hat{G}$ to real representations. But it must be unitary, to conserve the norm of any Hilbert space vector and thus the quantum probabilities:

$$|\psi\rangle \rightarrow \hat{G}|\psi\rangle, \quad \langle \psi | \rightarrow \langle \psi | \hat{G}^\dagger,$$

$$\langle \psi | \psi \rangle \rightarrow \langle \psi | \hat{G}^\dagger \hat{G} | \psi \rangle = \langle \psi | \hat{G}^{-1} \hat{G} | \psi \rangle = \langle \psi | \hat{1} | \psi \rangle = \langle \psi | \psi \rangle. \quad (2)$$

The particular representations of any $G$ can be simplified into irreducible representations (irreps). Such a representation is a vector space, typically a multidimensional subspace of $\mathcal{H}$, and defined in this way: an arbitrary group transformation $\hat{G}$ cannot map a vector lying in an irrep to a new vector lying outside that irrep subspace. Any arbitrary representation of a group is also a vector subspace in $\mathcal{H}$ and can always be decomposed into a linear combination of vectors lying in different irreps.

The fundamental group of quantum mechanics is the one-dimensional group of time evolution, generated by the Hamiltonian itself. Since the energy is conserved in a Hamiltonian system, a state that starts initially in a definite energy eigenstate $|E_n\rangle$ always remains...
in that state, apart from an exponential phase that carries the time dependence: \( |\psi(0)\rangle = |E_n\rangle \), so

\[
|\psi(t)\rangle = \exp[-i\hat{H}t/\hbar]|\psi(0)\rangle = \exp[-i\hat{H}t/\hbar]|E_n\rangle = e^{-iE_nt/\hbar}|E_n\rangle .
\]  

(3)

If the state is initially a linear combination, or superposition, of energy eigenstates, it can be written as

\[
|\psi(t)\rangle = \exp[-i\hat{H}t/\hbar]|\psi(0)\rangle = \exp[-i\hat{H}t/\hbar] \sum_n c_n |E_n\rangle = \sum_n c_n e^{-iE_nt/\hbar}|E_n\rangle .
\]  

(4)

If \( \hat{A} \) acts as a generator of a continuous group operation, a unitary group operation \( \hat{G} \) can be written as \( \hat{G} = \exp[i\alpha \hat{A}] \), where \( \alpha \) is a parameter that maps out the continuous manifold of the group transformations. (For a group transformation with multiple generators \( \{\hat{A}_a\} \), just replace \( \alpha \hat{A} \rightarrow \alpha_a \hat{A}_a \).) The group action on an operator is: \( \hat{B} \rightarrow \hat{G} \hat{B} \hat{G}^{-1} \).

If \( \hat{A} \) commutes with the Hamiltonian \( \hat{H} \), the transformation of the state vector \( |\psi(t)\rangle \) is

\[
\hat{G}|\psi(t)\rangle = \hat{G} \cdot \exp[-i\hat{H}t/\hbar]|\psi(0)\rangle = \hat{G} \cdot \exp[-i\hat{H}t/\hbar] \cdot \hat{G}^{-1} \hat{G}|\psi(0)\rangle
\]

\[
= \exp[i\alpha \hat{A}] \cdot \exp[-i\hat{H}t/\hbar] \cdot \exp[-i\alpha \hat{A}] \cdot \hat{G}|\psi(0)\rangle
\]

\[
= \exp[i\alpha \hat{A}] \cdot \exp[-i\hat{H}t/\hbar] \cdot \hat{G}|\psi(0)\rangle
\]

\[
= \hat{G} \hat{G}^{-1} \cdot \exp[-i\hat{H}t/\hbar] \cdot \hat{G}|\psi(0)\rangle = \exp[-i\hat{H}t/\hbar] \cdot \hat{G}|\psi(0)\rangle .
\]  

(5)

The penultimate line follows from \( [\hat{A}, \hat{H}] = 0 \). So the transformed initial state evolves to the transformed later state.

If \( \hat{A} \) is a generator of some \( \mathcal{G} \), the eigenstates of \( \hat{A} \) can be grouped into the irreps of \( \mathcal{G} \). If \( \hat{A} \) commutes with \( \hat{H} \), furthermore, eigenstates of one can be eigenstates of the other. We label eigenstates with both eigenvalues, \( |E_n, a_i\rangle \). If an initial state is an energy eigenstate and lies in an irrep of \( \mathcal{G} \), \( |\psi(0), n\rangle = \sum_i c_i |E_n, a_i\rangle \), the later state will always lie in that irrep, although not necessarily identical to the original state with just an additional phase. Following (5), the transformed later state is:

\[
\hat{G}|\psi(t)\rangle = \hat{G} \cdot \exp[-i\hat{H}t/\hbar]|\psi(0)\rangle = \hat{G} \exp[-iE_nt/\hbar] \hat{G}^{-1} \cdot \hat{G} \sum_i c_i |E_n, a_i\rangle
\]

\[
= \hat{G} \hat{G}^{-1} e^{-iE_nt/\hbar} \sum_i \exp[i\alpha \hat{A}] c_i |E_n, a_i\rangle = e^{-iE_nt/\hbar} \sum_i e^{i\alpha a_i} c_i |E_n, a_i\rangle .
\]  

(6)

The state is transformed by the overall phase associated with time evolution, but is also a linear combination (a linear combination different from the initial state) of eigenstates \( |E_n, a_i\rangle \) within the irrep.

The consequences of group theory for quantum mechanics were first examined by Weyl in the late 1920s. The general theoretical treatment was exhaustively worked out by Wigner in the 1930s.

2. Example: Parity in One Dimension

The simplest non-trivial group is the Abelian \( Z_2 \), switching two objects. A dynamical realization is parity. This operation changes all vectors to their negative (\( \mathbf{x} \rightarrow -\mathbf{x}, \mathbf{p} \rightarrow -\mathbf{p} \), etc.), but leaves pseudo-vectors (cross products in three dimensions) invariant. Thus, angular momentum \( \mathbf{L} = \mathbf{x} \times \mathbf{p} \) is left unchanged by the parity operation.
Parity is especially simple in one dimension, \( x \to -x \). The classical Lagrangian \( L = T(\dot{x}) - V(x) \) and Hamiltonian \( H = T(\dot{x}) + V(x) \) are invariant under parity if \( V(x) \) is. Classically, the motion in a parity-invariant bound potential (one in which the potential rises without limit as \( |x| \to \infty \)) is necessarily symmetrical around \( x = 0 \), the one point in space invariant under the parity operation.

The consequences in quantum mechanics are more interesting. There is a unitary parity operator \( \hat{P} \), satisfying \( \hat{P}^2 = 1 \), since the double action of parity is to take the system back to its original configuration. From Cayley’s theorem for matrices and linear operators, operators satisfy the same characteristic equation as their eigenvalues. Thus the eigenvalues of \( \hat{P} \) are \( \pm 1 \). These eigenvalues label eigenstates of even and odd parity.

In the position representation for the state vector, the state is described by a wave-function \( \psi(x, t) = \langle x | \psi(t) \rangle \). The position basis is a complete orthonormal set:

\[
\hat{x}|x\rangle = x|x\rangle \quad , \quad \langle x'|x\rangle = \delta(x-x') \quad , \quad \int_{-\infty}^{+\infty} dx \ |x\rangle \langle x| = \mathbf{1}
\]

Remove the time dependence in energy eigenstates by writing \( \psi(x, t) = e^{-iE_t/\hbar}\psi(x; E) \). The \( \psi(x; E) \) are the energy eigenstates and, for bound systems, come as a discrete set, with a discrete spectrum \( \{E_n\} \). Since \( [\hat{P}, \hat{H}] = 0 \), energy eigenstates are also parity eigenstates. That is, each \( \psi_n(x) \) has a definite parity: \( \psi_n(-x) = \pm \psi_n(x) \). The expectation value of \( \hat{x} \) is always zero in a parity eigenstate:

\[
\langle x \rangle = \langle n | \hat{x} | n \rangle = \int_{-\infty}^{+\infty} dx \cdot x \cdot |\psi_n(x)|^2 = 0 . \tag{7}
\]

Because \(|\psi_n(x)|^2 \) is even under \( x \to -x \) and \( x \) itself is odd, this integral must vanish.

The expectation value of \( \hat{x} \) does not vanish in general, in a superposition of energy eigenstates: \(|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |n\rangle \), and

\[
\langle x \rangle = \langle \psi(t) | \hat{x} | \psi(t) \rangle = \sum_{jk} c_j^* c_k e^{-i(E_k - E_j) t/\hbar} \langle j | \hat{x} | k \rangle
\]

\[
= \sum_{jk} c_j^* c_k e^{-i(E_k - E_j) t/\hbar} \int_{-\infty}^{+\infty} dx \ \psi_j^*(x) \cdot x \cdot \psi_j(x) . \tag{8}
\]

The matrix element \( x_{jk} = \langle j | \hat{x} | k \rangle \) vanishes if \(|i\rangle \) and \(|j\rangle \) have the same parity and, in particular, if \( j = k \). But if \(|j\rangle \) and \(|k\rangle \) have opposite parities, \( x_{jk} \) can be non-zero.

The simplest parity-invariant bound potential is the linear harmonic oscillator (LHO), \( V(x) = (1/2)m\omega^2x^2 \), where \( \omega \) is the angular frequency of the oscillator. (Its frequency is \( \nu = \omega/2\pi \).) There is a discrete infinity of energy eigenstates \(|n\rangle \) or \( \psi_n(x) \), with \( E_n = (n + 1/2)\hbar \omega \), \( n = 0, 1, 2, \ldots \). The parity of each \( \psi_n(x) \) is \((-1)^n : \psi_n(x) \) is even under reflection if \( n \) is even and odd if \( n \) is odd.

The expectation value \( \langle x \rangle \) simplifies for the LHO: \( x_{jk} = \langle j | \hat{x} | k \rangle \neq 0 \) only if \( j, k \) differ by one: \( k = j \pm 1 \). On dimensional units grounds, \( \langle x \rangle \) must be proportional to \( \sqrt{\hbar/m\omega} \), so write

\[
x_{jk} = \sqrt{\frac{\hbar}{m\omega}} \cdot [\delta_{j,k-1} \cdot D_-(j) + \delta_{j,k+1} \cdot D_+(j)] . \tag{9}
\]

Since \( \langle j | \hat{x} | j+1 \rangle = (j+1)|\hat{x}|j\rangle^* \propto (j+1)|\hat{x}|j-1\rangle \), \( D_+(j) = D_-(j) \equiv D(j) \). Furthermore, \( E_j - E_k = \mp \hbar \omega \), so

\[
\langle x \rangle = \frac{1}{2} \sqrt{\frac{\hbar}{m\omega}} \left\{ \left[ \sum_j c_j c_j^* \cdot D(j) \right] \cdot e^{+i\omega t} + \left[ \sum_j c_{j-1} c_j^* \cdot D^*(j) \right] \cdot e^{-i\omega t} \right\}
\]

\[
= \sqrt{\frac{\hbar}{m\omega}} \left\{ \Re \left[ \sum_j c_j c_j^* \cdot D(j) \right] \cdot \cos(\omega t) - \Im \left[ \sum_j c_j c_j^* \cdot D(j) \right] \cdot \sin(\omega t) \right\} , \tag{10}
\]
a general harmonic form identical to the classical motion:

\[ x(t) = C \cdot \cos(\omega t + \phi) = C \cdot [\cos \omega t \cdot \cos \phi - \sin \omega t \cdot \sin \phi] \quad , \]

\[ C = \sqrt{\frac{\hbar}{m\omega}} |\sum_j c_j c^*_j \cdot D(j)| \quad , \quad \tan \phi = \frac{\text{Im}\left[\sum_j c_j c^*_j \cdot D(j)\right]}{\text{Re}\left[\sum_j c_j c^*_j \cdot D(j)\right]} \quad . \tag{11} \]

But note that we needed a superposition of energy/parity eigenstates in (8) to arrive at this result. The transition (off-diagonal) matrix elements \( \langle j \mid \hat{x} \mid j \pm 1 \rangle \) are crucial.

The LHO, like the free particle and the Coulomb or Kepler potential, is an exactly solvable system in both quantum and classical mechanics, and the analogies between the quantum and classical solutions are close. Unfortunately, no other quantum or classical system is exactly solvable, and the quantum-classical correspondence is not as close in these other cases. Nonetheless, classical motion always results from superpositions of and transitions between energy eigenstates, with the time behavior of expectation values \( \langle A \rangle \) governed by differences in energies (8).

Since parity is a discrete symmetry, Noether’s theorem does not apply. There is still a “conserved” label (parity eigenvalue \( \pm 1 \)) for the quantum states. Such a number is called a good quantum number. Group theory is more general in quantum mechanics than in classical mechanics, partly because of the non-trivial representations of discrete symmetries.

3. Perturbation Theory and Selection Rules

If a quantum system starts in an eigenstate of a conserved operator \( \hat{A} \), it will remain in that eigenstate forever. But this property is true for an entire irrep subspace: if \( \langle \psi(0) \rangle \) lies in the irrep of \( \mathcal{G} \), the state never leaves that irrep, although it moves around in the subspace. The probability of changing to a different subspace at later times vanishes:

\[ \langle \text{irrep}_j | \psi(t) \rangle = \langle \text{irrep}_j | \text{exp}[-i\hat{H}t/\hbar] | \text{irrep}_j \rangle = e^{-iE_n t/\hbar} \langle \text{irrep}_j | \text{irrep}_j \rangle = 0 \quad . \]

This dynamical separation of irreps and conserved eigenvalues is called a superselection rule in quantum mechanics.

A further illustration of the power of group theory in quantum mechanics arises even if a Hamiltonian \( \hat{H} \) is not invariant under the group operation: \( \mathcal{G}\hat{H}\mathcal{G}^{-1} \neq \hat{H} \). Often in such cases, the part of \( \hat{H} \) that violates the symmetry is small compared to the rest of \( \hat{H} \). So split \( \hat{H} = \hat{H}_0 + \hat{H}_1 \), where \( \hat{H}_1 \) is a small perturbation. Now assume that for “small enough” \( \hat{H}_1 \) and time \( t \), any physical quantity the state can be expanded in a Taylor series in \( \hat{H}_1 \). This expansion is perturbation theory, which comes in two kinds.

Time-independent perturbation theory seeks the eigenvalues \( E_n \) and eigenvectors \( |E_n\rangle \) of the full \( \hat{H} \) in terms of the unperturbed eigenvalues \( E_n^{(0)} \) and eigenvectors \( |E_n^{(0)}\rangle \). The unperturbed energy spectrum and eigenstates serve as the zeroth-order starting point of the expansion. To first order in the expansion,

\[ E_n \doteq E_n^{(0)} + E_n^{(1)} \quad , \quad E_n^{(1)} = \langle E_n | \hat{H}_1 | E_n \rangle \quad . \tag{12} \]

Time-dependent perturbation theory seeks the time evolution governed by \( \hat{H} \) in terms of the eigenvalues and eigenvectors of \( \hat{H}_0 \). If \( |\psi(0)\rangle \) is an eigenstate \( |E_k^{(0)}\rangle \) of \( \hat{H}_0 \), \( \hat{H}_1 \) causes \( |\psi(t)\rangle \) to make transitions to other unperturbed eigenstates \( |E_k^{(0)}\rangle \); that is, to become a superposition of different \( |E_k^{(0)}\rangle \). Similarly, if \( \hat{H}_0 \) respects a symmetry \( \mathcal{G} \) and \( \hat{H}_1 \) does not,
an initial $|\psi(0)\rangle$ that is in an irrep subspace of $\mathcal{G}$ makes transitions to other irreps and become a superposition of different irreps over time.

Define the unperturbed time-evolution operator $\hat{U}_0(t) = \exp[-i\hat{H}_0 t/\hbar]$, an auxiliary state vector $|\psi'(t)\rangle = \hat{U}_0^{-1}(t)|\psi(t)\rangle$ that has the unperturbed time evolution removed, and an auxiliary perturbation Hamiltonian $\hat{H}_1(t) = \hat{U}_0^{-1}(t)\hat{H}_1\hat{U}_0(t)$ that is transformed to evolve backwards with the unperturbed $\hat{H}_0$. Let $\omega_{ij} \equiv [E_i^{(0)} - E_j^{(0)}]/\hbar$ be the quantum transition frequency between unperturbed eigenstates $|E_i^{(0)}\rangle$ and $|E_j^{(0)}\rangle$. Then the perturbation evolution and its formal solution are:

$$\frac{i\hbar}{\partial t}|\psi'(t)\rangle = \hat{H}_1'(t)|\psi'(t)\rangle \quad , \quad |\psi'(t)\rangle = \hat{V}_1(t)|\psi'(0)\rangle = \hat{V}_1(t)|\psi(0)\rangle \quad ,$$

$$\hat{V}_1(t) = \hat{1} - \frac{i}{\hbar}\int_0^t \hat{H}_1'(t')dt' + \left(-\frac{i}{\hbar}\right)^2\int_0^t \hat{H}_1'(t')dt'\int_0^{t'} \hat{H}_1''(t'')dt'' + \cdots .$$

If $|\psi(0)\rangle = |E_n^{(0)}\rangle$, the transition amplitude from $|E_n^{(0)}\rangle$ to another unperturbed eigenstate $|E_k^{(0)}\rangle$ as a function of time is then

$$\langle k|\psi(t)\rangle = \delta_{kn} - \frac{i}{\hbar}\int_0^t \langle k|\hat{H}_1|n\rangle e^{i\omega_n t} + \mathcal{O}(\hat{H}_1^2) .$$

The transition probability $P(n \rightarrow k; t)$ is the norm-squared of this amplitude.

Consider perturbing the LHO quadratic potential with a small linear term: $V(x) \rightarrow (1/2)m\omega^2x^2 + bx$, with $|b| \ll m\omega^2(x)$. The system can no longer be solved exactly, and the exact parity symmetry is lost. In the previous section, we evaluated the $\langle k|\hat{H}_1|n\rangle$, so we reuse that result. The first-order energy eigenvalue correction $E_n^{(1)}$ vanishes by parity symmetry: $E_n^{(1)} = b \cdot \langle n|\hat{x}|n\rangle = 0$.

The transition amplitude to another unperturbed LHO eigenstate $|k\rangle$ is

$$P(n \rightarrow k; t) = \delta_{kn} - \frac{i}{\hbar} \cdot b \cdot \sqrt{\frac{\hbar}{m\omega}}\int_0^t \left[ \delta_{k,n-1} \cdot D^*(k)e^{-i\omega t} + \delta_{k,n+1} \cdot D(k)e^{i\omega t} \right] dt .$$

At this order, from (14), $P(n \rightarrow k; t) = 1$ if $k = n$,

$$P(n \rightarrow k; t) = \frac{2b^2}{\hbar m\omega^3} \cdot |D(k)|^2 \cdot [1 - \cos \omega t]$$

if $k = n \pm 1$, and all other other transitions vanish. The cosine term is usually eliminated by averaging over a period $2\pi/\omega$.

Any unperturbed parity-symmetric system with a parity-violating perturbation $\hat{H}_1$ would make such parity-changing transitions at first order in perturbation theory. Even though the full $\hat{H}$ violates parity, the underlying space $x \in (-\infty, +\infty)$ is parity-symmetric. A matrix element is non-zero only if the entire integrand $\psi^*_k \cdot x \cdot \psi^*_n$ has even parity. The functions $\psi_{k,n}(x)$ have definite parity. The operator $\hat{x}$ is parity-odd, $\hat{P}\hat{x}\hat{P}^{-1} = -\hat{x}$. Ergo, states $k$ and $n$ must have opposite parity to have a non-zero matrix element. Such transitions are *allowed*, while, at this order, parity-conserving transitions are *forbidden*. At higher orders, the parity-conserving transitions actually do occur but are *suppressed* for small $\hat{H}_1$. Parity symmetry controls which transitions take place, even though the parity symmetry is violated by the full $\hat{H}$!

Transition rules of this type are called *selection rules* in quantum mechanics. They rely on the fact that not only do the unperturbed eigenstates $|E_n^{(0)}\rangle$ lie in irreps of $\mathcal{G}$, the
perturbation operators $\hat{H}_1$ themselves usually lie in definite irreps of $\mathcal{G}$. These irreps are just not trivially invariant: $\hat{P}\hat{H}_0\hat{P}^{-1} = +\hat{H}_0$, but $\hat{P}\hat{H}_1\hat{P}^{-1} = -\hat{H}_1$ in the perturbed LHO example. The non-invariance of the perturbation causes the transitions, but its irrep-ness forces the transitions to follow selection rules.

This simple example illustrates again the power of group theory in quantum mechanics even when symmetries are not exactly respected. The analysis of exact and approximately exact symmetries leads to selection rules that are applicable in atomic, molecular, nuclear, and elementary particle systems, as well as meso- and macroscopic quantum systems such as semiconductors, laser optic cables, and superconductors and superfluids.

**Note on the Dirac Delta Function**

The Dirac delta function $\delta(x)$ is formally defined as:

$$\delta(x) = 0 \text{ if } x \neq 0 ; \quad \int_{-\epsilon}^{+\epsilon} dx \delta(x) = 1 ; \quad f(0) = \int_{-\epsilon}^{+\epsilon} dx \, f(x)\delta(x) ,$$

for $\epsilon \to 0^+$, and any smooth function $f(x)$. An equivalent definition in terms of the Heaviside “step” function $\theta(x)$ is $\delta(x) \equiv \theta'(x)$, where

$$\theta(x) \equiv \begin{cases} 
0, & \text{if } x < 0; \\
1, & \text{if } x > 0.
\end{cases}$$

The result in terms of Fourier analysis is:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \, e^{ikx} .$$

The delta function is actually a distribution, the limit of a sequence of functions:

$$\delta(x) \equiv \lim_{a \to 0} \frac{a}{\pi} \sin(x/a) \quad \text{or} \quad \lim_{b \to 0} \frac{b}{\pi x^2 + b^2}$$

or

$$\lim_{c \to 0} \frac{1}{c\sqrt{\pi}} e^{-x^2/c^2} \quad \text{or} \quad \lim_{z \to 0} \begin{cases} 
1/z, & \text{if } |x| \leq z/2, \\
0, & \text{if } |x| > z/2.
\end{cases}$$

The Dirac delta function serves the role in continuous vector spaces that the Kronecker delta $\delta_{ij}$ serves in discrete spaces.
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Short Bibliography

Dallas C. Kennedy · · · The MathWorks, Inc.


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