

Chapter 1

Nonrelativistic Quantum Mechanics

In this Lecture nonrelativistic quantum mechanics is reviewed briefly following an approach originally due to Dirac.

1.1 Lagrangian and Hamiltonian Mechanics

The most convenient form of classical mechanics as a basis for generalization to quantum mechanics is Hamiltonian mechanics. Starting from a Lagrangian system, Hamilton's equations are introduced by making a Legendre transformation, that is, by changing the independent variables.

In Lagrangian mechanics, a holonomic system with s degrees of freedom is described by a set of s generalized coordinates q_1, \dots, q_s and the associated generalized velocities $\dot{q}_1, \dots, \dot{q}_s$, where the dots denote the time derivatives. The Lagrangian $L(q, \dot{q}, t)$ is a function of these variables, where q and \dot{q} denote, respectively, q_1, \dots, q_s and $\dot{q}_1, \dots, \dot{q}_s$ collectively. The equations of motion in Lagrangian form are

$$\left[\frac{d}{dt} \frac{\partial}{\partial \dot{q}_i} - \frac{\partial}{\partial q_i} \right] L(q, \dot{q}, t) = 0, \quad \text{for } i = 1, \dots, s. \quad (1.1)$$

The generalized momenta p_1, \dots, p_s are defined by

$$p_i := \frac{\partial}{\partial \dot{q}_i} L(q, \dot{q}, t), \quad i = 1, \dots, s. \quad (1.2)$$

The change of independent variables is from the q and \dot{q} to the q and p . If one writes

$$H = \sum_{i=1}^s p_i \dot{q}_i - L, \quad (1.3)$$

then in the differential

$$dH = \sum_{i=1}^s \left\{ p_i d\dot{q}_i + \dot{q}_i dp_i \right\} - \sum_{i=1}^s \left\{ \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i \right\}$$

the terms involving $d\dot{q}_i$ cancel, so that the q and p are the new independent variables, as required. The equations of motion (1.1) and the relation implied by (1.3) between the \dot{q} and p become

$$\dot{q}_i = \frac{\partial}{\partial p_i} H(q, p, t), \quad \dot{p}_i = -\frac{\partial}{\partial q_i} H(q, p, t), \quad \text{for } i = 1, \dots, s. \quad (1.4)$$

These are Hamilton's equations.

1.2 Canonical Transformations and Poisson Brackets

Within the framework of classical mechanics, a major advantage of the Hamiltonian formalism over the Lagrangian formalism is the ability to make *canonical transformations*. Such a transformation is from variables q, p and Hamiltonian $H(q, p)$ to another set of variables Q, P and Hamiltonian $K(Q, P)$, where Q and P are functions of q and p . The new variables and the new Hamiltonian satisfy Hamilton's equations.

A special case of a canonical transformation is a *point transformation*, which corresponds to the new coordinates Q being functions only of the old coordinates q , and not of the old momenta p . The new Hamiltonian is then equal to the old Hamiltonian. A simple example of a point transformation is the transformation from cartesian to spherical polar or cylindrical polar coordinates. Note that, although the new coordinates do not depend on the old momenta, the new momenta do depend on the old coordinates as well as on the old momenta in general; for example, the radial momentum in spherical polar coordinates is $p_r = (xp_x + yp_y + zp_z)/r$.

The detailed form of Hamilton's equations depends on the choice of coordinates (and on the choice of gauge in the presence of an electromagnetic field). It is desirable to develop much of the theory in a way that is independent of the specific choices made. One such development is based on the use of Poisson brackets. Let f and g be any functions of q, p, t . Their Poisson bracket is defined by

$$[f, g]_{\text{P}} := \sum_{i=1}^s \left[\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right]. \quad (1.5)$$

The value of $[f, g]_{\text{P}}$ is unchanged under a canonical transformation.

Setting f and g equal to one of the q or p leads to the *fundamental Poisson brackets*

$$[q_i, q_j]_{\text{P}} = 0, \quad [p_i, p_j]_{\text{P}} = 0, \quad [q_i, p_j]_{\text{P}} = \delta_{ij}, \quad i, j = 1, \dots, s. \quad (1.6)$$

These relations may be reinterpreted as a definition of a canonical set (q, p). Also the time evolution of any function is determined by its explicit

time dependence and its Poisson bracket with the Hamiltonian:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_{i=1}^s \left[\dot{q}_i \frac{\partial f}{\partial q_i} + \dot{p}_i \frac{\partial f}{\partial p_i} \right] = \frac{\partial f}{\partial t} + [f, H]_{\text{P}}, \quad (1.7)$$

where (1.4) and (1.5) are used.

1.3 The State Function and Operators

There are several steps in the generalization from classical mechanics to quantum mechanics. Firstly a conceptual change needs to be made. This involves describing the particular system of interest in terms of a state function.

To allow for interference and diffraction effects, one needs to introduce a representation of a state of a system that can be decomposed into two or more parts that can interfere with each other. Dirac introduced such a state function in an abstract way in terms of his bra, $\langle |$, and ket, $| \rangle$, notation. What is known about the system is included in the state function, and it is convenient to include this information as arguments, so that $|1\rangle$ and $|2\rangle$ describe states labelled 1 and 2, respectively. The ket $| \rangle$ is regarded as a vector in a complex vector space, specifically a Hilbert space \mathcal{H} , and the corresponding bra $\langle | = \{ | \rangle \}^\dagger$ as the corresponding vector in the adjoint Hilbert space \mathcal{H}^\dagger (in which all quantities are complex conjugated). The ket for a mixed state (such as in a two slit diffraction experiment) is the sum of the kets for the states of which it is composed.

The inner product is a bracket formed from a bra and a ket. The inner product between states 2 and 1 is written

$$\langle 2|1\rangle = \langle 1|2\rangle^*$$

where $*$ denotes complex conjugation.

One extracts information on the system by performing a set of operations (measurements or observations) on the system. Each set of operations is described by an operator in the Hilbert space. Operators are denoted by hats, with \hat{Q} the operator corresponding to measuring a quantity Q . An operation can change the state of a system. The number

$$Q_{21} = \langle 2|\hat{Q}|1\rangle \quad (1.8)$$

is referred to as the *matrix element* between states 1 and 2 for the operator \hat{Q} . If the operation of \hat{Q} on a system leads to a definite value Q , then the system is in an eigenstate of \hat{Q} with eigenvalue Q . Observable values are real numbers, and hence the eigenvalues of an observable quantity must be real. This requires that the operators corresponding to observable quantities be self adjoint: $\hat{Q}^\dagger = \hat{Q}$.

Two other formal requirements are that the eigenkets of any self adjoint operator span the Hilbert space, and that eigenkets corresponding to different eigenvalues be orthogonal. For continuous eigenvalues this orthogonality condition led Dirac to introduce the δ -function. Thus if q and q' are two different eigenvalues of an operator \hat{q} with a continuous spectrum of eigenvalues, then one requires

$$\langle q' | \hat{q} | q \rangle = q \delta(q - q'). \quad (1.9)$$

These ideas are summarized in the following axioms:

The state of a system is described by a vector (a ket $| \rangle$) in a Hilbert space \mathcal{H} , and an observable Q is described by a self adjoint operator \hat{Q} in \mathcal{H} . The eigenkets of any self adjoint operator span the Hilbert space, and eigenkets corresponding to different eigenvalues are orthogonal.

The link between this formalism and the classical description is expressed in terms of the relation between the quantum mechanical commutator between two operators and the corresponding Poisson bracket. The commutator is

$$[\hat{f}, \hat{g}] = \hat{f} \hat{g} - \hat{g} \hat{f}. \quad (1.10)$$

The relation is expressed in the following axiom (retaining \hbar explicitly for the present):

The commutator $[\hat{f}, \hat{g}]$ of any two operators is equal to $i\hbar$ times the corresponding Poisson bracket $[f, g]_{\text{P}}$.

The basic Poisson brackets (1.6) then imply the *fundamental commutation relations*

$$[\hat{q}_i, \hat{q}_j] = 0, \quad [\hat{p}_i, \hat{p}_j] = 0, \quad [\hat{q}_i, \hat{p}_j] = i\hbar \delta_{ij}, \quad i, j = 1, \dots, s. \quad (1.11)$$

1.4 Representations

In detailed calculations it is usually convenient to use a specific representation of the Hilbert space. The most widely used representation is the *coordinate* or *Schrödinger* representation. This representation is implicit in the familiar Schrödinger equation of nonrelativistic quantum mechanics, and in the standard forms for the Klein Gordon and Dirac equations. Other representations include the momentum representation, which is related to the coordinate representation by a Fourier transform and is sometimes useful when plane wave solutions are involved, and matrix representations, which are useful when the eigenvalues are discrete.

The coordinate representation is introduced by using the eigenkets $|q\rangle$ ($= |q_1, \dots, q_s\rangle$) of the coordinate operators \hat{q}_i as basis vectors in the Hilbert space. One has

$$\hat{q}_i |q_1, \dots, q_s\rangle = q_i |q_1, \dots, q_s\rangle, \quad i = 1, \dots, s. \quad (1.12)$$

The matrix elements of the coordinate operators are diagonal:

$$\langle q'_1, \dots, q'_s | \hat{q}_i | q_1, \dots, q_s \rangle = q_i \delta(q_1 - q'_1) \dots \delta(q_s - q'_s), \quad (1.13)$$

and this implies that the operator \hat{q}_i is represented by multiplication by q_i . An arbitrary ket $| \rangle$ is represented by the so called wavefunction

$$\Psi(q) = \langle q | \rangle, \quad (1.14)$$

where the argument q represents q_1, \dots, q_s collectively. Finally, to satisfy the commutation relations (1.11), the operator \hat{p}_i must be represented by $-i\hbar\partial/\partial q_i$.

1.5 Pictures for the Time Evolution

A final major step in generalizing classical mechanics to quantum mechanics involves including the time evolution. The classical evolution of any variable f may be described in the form (1.7). To avoid possible confusion, let us assume that f does not depend explicitly on time ($\partial f/\partial t = 0$). Then the classical evolution of f is due only to the dependence of f on the changing coordinates and momenta of the particles in the system. We are concerned with the quantum mechanical counterpart of this evolution.

In quantum mechanics f is replaced by the matrix elements of the corresponding operator \hat{f} , and one is free to choose to include the time evolution in the operator or in the kets and bras, or in a mixture of the two. All three choices are convenient for different purposes. Any specific choice is referred to as a *picture* for the time evolution. The *Schrödinger picture* has all the time evolution in the kets and bras, and the *Heisenberg picture* has all the evolution in the operators. The *interaction picture* has part of the evolution in the bras and kets and another part in the operators.

Note that the some authors refer to *representations* of the time evolution. Here *representation* is used only to refer to representations of the kets and operators in the Hilbert space, and *picture* is used exclusively to refer to the time evolution.

In the Schrödinger picture the operators do not depend on time and the evolution of the kets implied by (1.7), with the Poisson bracket replaced by the commutator as postulated, is

$$i\hbar \frac{d}{dt} |t\rangle_S = \hat{H} |t\rangle_S, \quad (1.15)$$

where the subscript S denotes the Schrödinger picture. In the Heisenberg picture the kets do not depend on time and the operators evolve according to

$$i\hbar \frac{d}{dt} \hat{f}_H = [\hat{f}_H, \hat{H}], \quad (1.16)$$

where the subscript H denotes the Heisenberg picture.

1.6 The Schrödinger Equation

The Schrödinger equation applies in the Schrödinger picture and the coordinate representation. Writing $H(q, p, t)$ for the Hamiltonian, including only one coordinate explicitly, the coordinate representation of (1.15) becomes

$$\left[i\hbar \frac{\partial}{\partial t} - \hat{H}(q, -i\hbar\partial/\partial q, t) \right] \Psi(q, t) = 0, \quad (1.17)$$

which is a general form of the *Schrödinger equation*.

The specific systems of interest here are a free particle and a particle in an electromagnetic field. The Hamiltonian for a nonrelativistic free particle is $H = \mathbf{p}^2/2m$, in which case (1.17) becomes

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right] \Psi(\mathbf{x}, t) = 0, \quad (1.18)$$

with

$$\nabla^2 = \text{div grad} = (\partial/\partial x)^2 + (\partial/\partial y)^2 + (\partial/\partial z)^2.$$

The Hamiltonian for a nonrelativistic particle with charge q in an electromagnetic field is $H = (\mathbf{p} - q\mathbf{A})^2/2m + q\phi$. Then (1.18) is replaced by

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - \frac{i\hbar q}{m} \mathbf{A} \cdot \text{grad} - \frac{i\hbar q}{2m} \text{div} \mathbf{A} + \frac{q^2}{2m} \mathbf{A}^2 + q\phi \right] \Psi(\mathbf{x}, t) = 0. \quad (1.19)$$

The prescription for generalizing relativistic Hamiltonians to include the electromagnetic field is analogous to the nonrelativistic case: \mathbf{p} is replaced by $\mathbf{p} - q\mathbf{A}$ and a term $q\phi$ is added to H .

1.7 Inclusion of Spin

The spin of the electron needs to be included artificially in the generalization of the Schrödinger equation to the Schrödinger-Pauli equation. One introduces a complex two dimensional spin space, thereby formally doubling the dimensionality of the Hilbert space, and introduces a spin vector $\frac{1}{2}\hbar\boldsymbol{\sigma}$ in this space. The Hamiltonian H for an electron is replaced by

$$H = H' - \mu_e \boldsymbol{\sigma} \cdot \mathbf{B}, \quad (1.20)$$

where

$$\mu_e = \frac{e\hbar}{2m} \quad (1.21)$$

is the magnetic moment of the electron.

The components of $\boldsymbol{\sigma}$ are the Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.22)$$

They satisfy the relations

$$\sigma_x \sigma_y + \sigma_y \sigma_x = 0, \quad \sigma_x \sigma_y = i \sigma_z, \quad (\sigma_x)^2 = 1, \quad (1.23)$$

together with other identities obtained by cyclic permutations of x, y, z . In tensor notation (1.23) becomes

$$\sigma_i \sigma_j = \delta_{ij} + i \varepsilon_{ijk} \sigma_k. \quad (1.24)$$