Preface

Quantum mechanics was already an old and solidly established subject when the first edition of this book appeared in 1966. The context in which a graduate text on quantum mechanics is studied today has changed a good deal, however. In 1966, most entering physics graduate students had a quite limited exposure to quantum mechanics in the form of wave mechanics. Today the standard undergraduate curriculum contains a large dose of elementary quantum mechanics, and often introduces the abstract formalism due to Dirac. Back then, the study of the foundations by theorists and experimenters was close to dormant, and very few courses spent any time whatever on this topic. At that very time, however, John Bell's famous theorem broke the ice, and there has been a great flowering ever since, especially in the laboratory thanks to the development of quantum optics, and more recently because of the interest in quantum computing. And back then, the Feynman path integral was seen by most as a very imaginative but rather useless formulation of quantum mechanics, whereas it now plays a large role in statistical physics and quantum field theory, especially in computational work.

For these and other reasons, this book is not just a revision of the 1966 edition. It has been rewritten throughout, is differently organized, and goes into greater depth on many topics that were in the old edition. It uses Dirac notation from the outset, pays considerable attention to the interpretation of quantum mechanics and to related experiments. Many topics that did not appear in the 1966 edition are treated: the path integral, semiclassical quantum mechanics, motion in a magnetic field, the S matrix and inelastic collisions, radiation and scattering of light, identical particle systems and the Dirac equation.

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Kurt Gottfried has here, at last, the opportunity to thank colleagues who have, either in writing or face-to-face, shared their knowledge, patiently answered questions and corrected misconception: in particular Aage Bohr, Michael Berry, Roy Glauber, Daniel Greenberger, Martin Gutzwiller, Eric Heller, Michael Horne, Ben Mottelson, Michael Nauenberg, Abner Shimony, Ole Ulfbeck and Anton Zeilinger, and the late John Bell, Rudolf Peierls and Donald Yennie. He is deeply indebted to David Mermin and Yuri Orlov for innumerable enlightening and stimulating discussions over many years.

We both wish to take this occasion to thank and remember those who first taught us quantum mechanics: David Jackson, Julian Schwinger and Victor Weisskopf.

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January 2003

Road Signs

This book treats considerably more material than fits into a standard *two-semester* course. Furthermore, the rigid organization of this (or any) book does not map in a simply-connected manner onto a good course. We therefore offer some guidance based on our experience with what we have found suitable for the *first* semester. Personal judgments and interests should be used to select material for the second semester, or for self-instruction. Various selections have been taught by us in the first semester. The emphasis has been on physical phenomena, with the general theory and approximation techniques intermingled with applications. The last time the semester was confined to general theory as motivated and illustrated by various one-body problems:

- The portions of the first three chapter with which students are not yet familiar, but leaving almost all of § 2.6 - § 2.9 on propagators, the path integral and semiclassical quantum mechanics for later.
- Low Dimensional Systems: spectroscopy in two-level systems, the harmonic oscillator and motion in a magnetic field.
- Hydrogenic atoms: fine and hyperfine structure, and the Zeeman and Stark effects, i.e., most of chapter 5, leaving aside Pauli's solution (§ 5.2).
- Symmetries: the rotation group (§ 7.4), some consequences of rotational symmetry (part of § 7.5); and tensor operators (§ 7.6).
- Elastic Scattering: general theory (§ 8.1 – § 8.2), approximation methods (§ 8.3), and scattering of particles with spin (§ 8.5).

References. Complete citations are given in Endnotes and the text, except for the following which recur often and are denoted by abbreviations:

Bethe and Salpeter: *Quantum Mechanics of One- and Two-Electron Atoms,* H.A. Bethe and E.E. Salpeter, Springer-Verlag (1957)

Jackson: *Classical Electrodynamics*, J.D. Jackson, 3rd. ed., Wiley (1999)

LLQM: Quantum Mechanics, L.D. Landau and E.M. Lifshitz, 3rd. ed., Pergamon (1977)

WZ: *Quantum Theory and Measurement*, J.A. Wheeler and W.H. Zurek (eds.), Princeton (1982)

Equation numbering. Equations are numbered sequentially in each chapter, and those in different chapters are cited as $(n.m)$, where n is the number of the other chapter.

Errata. Corrections should be sent to both kg13@cornell.edu and ty18@cornell.edu. They will be posted on http://www.lepp.cornell.edu/books/QM-I/

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The Formal Framework

The concepts described impressionistically in chapter 1 must be cast into a well-defined mathematical formalism if one is to do theoretical physics. This chapter is devoted to a first cut at this task. Much of the material, such as that on symmetries and on the interpretation of quantum mechanics, will be reconsidered in greater depth in later chapters.

As in chapter 1, we assume that this is not the reader's first encounter with this material. Hence the presentation is occasionally terse, but as readers will have various levels of prior knowledge, it also seeks to be reasonably self-contained. One important point should be made at the outset. The level of mathematical rigor will be typical of the bulk of the theoretical physics literature — slovenly. Mathematicians view sloppy rigor as an oxymoron. Readers who share this view should consult the bibliography at the end of this chapter.

Any physical theory employs concepts more primitive than those on which the theory sheds light. In classical mechanics these primitive concepts are time, and points in three-dimensional Euclidean space. In terms of these, Newton's equations give unequivocal definitions of such concepts as momentum and force, which had only been qualitative and ambiguous notions before then. Maxwell's equations and the Lorentz force law, in conjunction with Newton's equations, define the concepts of electric and magnetic fields in terms of the motion of test charges.

There is no corresponding clearcut path from classical to quantum mechanics. In many circumstances, though certainly not all, classical physics tells us how to construct the appropriate Schrödinger equation that describes a particular phenomenon. But the statistical interpretation of quantum mechanics is not implied by the Schrödinger equation itself.[1] For this and other reasons the interpretation of quantum mechanics is still controversial despite its unblemished empirical success. In this chapter we therefore adopt a brashly pragmatic attitude to many issues concerning the interpretation of quantum mechanics, in the belief these matters are best pondered at length after combat experience, as they will be in chapter 12.

2.1 The Formal Language: Hilbert Space

The quantum state is a fundamentally abstract concept. For brevity, name it Ψ. Abstract concepts are also important in classical physics, but as mathematical and intuitive idealizations of concrete things. That is not so of the quantum state.

[1] This can be put as a fable. If Newton were to be shown Maxwell's equations and the Lorentz force law, he could figure out what is meant by the unfamiliar symbols $\boldsymbol{E}$ and $\boldsymbol{B}$, but if Maxwell was handed Schrödinger's equation he could not decipher the meaning of ψ. For an elaboration, see K. Gottfried, *Nature* **405**, 533 (2000).

The fact that any Ψ pertaining to an N-particle system can be given a numerical representation as a Schrödinger wave function $\psi(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N)$, whose variables are in good old configuration space, should not be read as implying that ψ is any more concrete than is Ψ. This warning is not just an ideological prejudice; if it is ignored one is led to seemingly plausible conceptions of reality that must be abandoned, as we will see in chapter 12.

In classical mechanics, the state of an N-particle system is specified by a point $X = (q_1 \ldots q_{3N}; p_1 \ldots p_{3N})$ in $6N$ dimensional phase space Ω_{qp}, where the q_j and p_j are the canonical coordinates and momenta. The equations of motion then specify how X moves about in Ω_{qp}. The states of all systems with $3N$ degrees of freedom inhabit this same space Ω_{qp}, with systems that have different forces and masses moving along different families of trajectories. Given X, all properties of the system are completely specified.

The quantum state Ψ differs from X in two ways: (i) it "lives" in an abstract space (Hilbert space) that has no connection to the "real" world; (ii) given a mathematical expression for Ψ, quantum mechanics provides unambiguous statistical predictions about the outcomes of all observations on the system that Ψ describes. There are analogies, on the other hand. The quantum states of all systems having the same degrees of freedom live in the same Hilbert space. And just as X gives a complete description in classical mechanics, so does Ψ in quantum mechanics, though of course the meaning of "complete" is very different.

Because quantum mechanics makes only statistical predictions in most circumstances, there is a tendency to overstate quantum mechanical uncertainty. In important ways, quantum mechanics provides more knowledge than does classical mechanics, a point that is often given short shrift. For example, if a monoatomic gas is in an environment that cannot impart enough energy to lift its atoms out of their ground state, we know all about it, so to say, no matter whether it is in a laboratory or in intergalactic space. That all these atoms have precisely the same ground state cannot be understood in classical mechanics.

The quantum state can be given a numerical form in an infinity of ways — by functions in the configuration space $\mathfrak{C}$, or in momentum space, to name just two. There is an analogy here to classical mechanics, where a description in terms of intuitively appealing variables can be translated into an infinity of others by canonical transformations. But phase space as a whole cannot be used to describe quantum mechanical probability distributions, because the uncertainty principle rules out simultaneous precise knowledge of coordinates and conjugate momenta.

Furthermore, wave-particle duality implies that Ψ cannot, over time, be strictly confined to any subspace $\mathfrak{C}$. At some instant it may be so confined, but thereafter it will spread, with finite speed in a quantum theory that complies with relativity, but instantaneously in nonrelativistic quantum mechanics. The whole setting in which the system can exist, in principle, is involved in defining Ψ. Restated with poetic license, a classical golfer whose ball leaves the tee flying toward a gap between two trees cares not one whit about their size, or about other trees that it will never encounter, whereas a quantum golfer does — "will never encounter" has no clear meaning for the quantum golfer.

(a) Hilbert Space

The elements of the language appropriate for describing quantum states in the configuration space $\mathfrak{C}$ are *complex* "wave" functions $\psi(q_1 \dots q_{3N})$. Any such function — whether or not it is a solution of some Schrödinger equation — can be specified uniquely in terms of a complete orthonormal set of functions. For the moment, let's restrict the range of all the coordinates to be finite, $-\frac{1}{2}L \le q_j \le \frac{1}{2}L$, with L larger than any physical dimension of interest, so that the volume of configuration space is L^{3N}. In this case such complete sets are denumerable: $u_a(q_1 \dots q_{3N}),\ a = 1, 2, \dots$. The term *complete* means that any ψ can be expressed as a linear combination of the u_a,

$$\psi(q_1 \dots q_{3N}) = \sum_{a=1}^{\infty} c_a u_a(q_1 \dots q_{3N}) \ . \tag{1}$$

The term *orthonormal* means that

$$\int dq_1 \dots dq_{3N}\ u_a^*(q_1 \dots q_{3N}) u_{a'}(q_1 \dots q_{3N}) \equiv \int (dq)\, u_a^*(q) u_{a'}(q) = \delta_{aa'} \ , \tag{2}$$

which also defines a convenient shorthand. As a consequence, the expansion coefficients c_a are

$$c_a = \int (dq)\, u_a^*(q) \psi(q) \ . \tag{3}$$

Substitution into the original expansion for ψ then produces the completeness relation for the set $\{u_a\}$:

$$\sum_a u_a(q) u_a^*(q') = \delta^{3N}(q - q') \ , \tag{4}$$

where now the shorthand means

$$\delta^{3N}(q - q') \equiv \prod_{j=1}^{3N} \delta(q_j - q_j') \ . \tag{5}$$

In these equations $\delta_{aa'}$ is the Kronecker delta, i.e., 1 or 0 according to whether a and a' are equal or not, and $\delta(x - x')$ the one-dimensional Dirac delta function, defined by the property

$$f(x) = \int \delta(x - x') f(x') dx'$$

for any function f that is continuous at x.

The set of square integrable functions $\{u_a(q)\}$ constitute a *basis* in an infinite-dimensional complex vector space, called a *Hilbert space* $\mathfrak{H}$. It is the space that plays a role akin to that of phase space in classical mechanics — the stage on which quantum mechanics performs.

The functions $u_a(q)$ on the configuration space $\mathfrak{C}$ do not form a unique description of this particular basis. Consider, for example, the Fourier transform of u_a:

$$v_a(p_1 \dots p_{3N}) \equiv v_a(p) = \prod_{j=1}^{3N} \int_{-\frac{1}{2}L}^{\frac{1}{2}L} \frac{dq_j}{\sqrt{L}}\, e^{-ip_j q_j/\hbar}\ u_a(q_1 \dots q_{3N}) \ , \tag{6}$$

where

$$p_j/\hbar = 2n_j\pi/L, \quad n_j = 0, \pm 1, \pm 2, \dots \ . \tag{7}$$

so that the functions $\Pi_j \exp(ip_jq_j/\hbar)$ satisfy periodic boundary conditions on the surface of $\mathfrak{C}$. At the moment, $\hbar$ is merely any constant having the dimension of action so as to make $p/\hbar$ an inverse length and to give p the dimension of momentum. The physical content required to make it Planck's constant has not yet entered the story.

Eq. 6 says that the set of functions $\{v_a(p)\}$ in momentum space provides a "representation" of the *same* basis in $\mathfrak{H}$ as does the set $\{u_a(q)\}$ in configuration space. This statement can be rephrased in a fruitful manner by noting that the plane waves form a complete orthonormal basis which is distinct from the one formed by the u_a (or equivalently, the v_a). That is, define

$$\phi_{p_1 \dots p_{3N}}(q_1 \dots q_{3N}) \equiv \phi_p(q) = \prod_{j=1}^{3N} \frac{e^{iq_jp_j/\hbar}}{\sqrt{L}} \ ; \tag{8}$$

then, as just claimed,

$$\int (dq)\, \phi_p^*(q)\phi_{p'}(q) = \prod_j \delta_{p_jp'_j} \equiv \delta_{pp'}^{3N} \ , \tag{9}$$

$$\sum_{p_1 \dots p_{3N}} \phi_p(q)\phi_p^*(q') = \delta^{3N}(q - q') \ . \tag{10}$$

In terms of this notation, Eq. 6 is

$$v_a(p) = \int (dq)\, \phi_p^*(q)u_a(q) \ , \tag{11}$$

and conversely, because of (9),

$$u_a(q) = \sum_{\{p\}} \phi_p(q)v_a(p) \ . \tag{12}$$

(b) Dirac's Notation

These somewhat unsightly expressions follow with seductive ease from a notation of great power due to Dirac. Notation is no laughing matter as Newton learned from his competitor Leibniz.

The basic idea, long familiar to mathematicians, is borrowed from vector algebra. Consider a real three-dimensional Euclidean space $\mathfrak{E}_3$. Any two vectors ($\boldsymbol{v}$, $\boldsymbol{w}$) can be described by an infinity of bases, and in particular, by any one of an infinity of distinct triads of mutually perpendicular unit vectors. Given such a basis, $\boldsymbol{v}$ and $\boldsymbol{w}$ can be specified by two triplets of real numbers, their projections onto the basis triad. However — and this is the crux of the matter, the geometrical meaning of $\boldsymbol{v}$ and $\boldsymbol{w}$, and of their scalar and vector product, are basis-independent: in all bases $\boldsymbol{v} \cdot \boldsymbol{w}$ is the same real number, and $\boldsymbol{v} \times \boldsymbol{w}$ is a vector perpendicular to both $\boldsymbol{v}$ and $\boldsymbol{w}$ and of a length that is basis-independent.

The generalization of these concepts appropriate to quantum mechanics is a d-dimensional complex vectors space — a Hilbert space if d is infinite; usually the

space will be denoted by $\mathfrak{H}$ in either case. In Dirac's nomenclature, the vectors in this space are called *kets*, and denoted by the symbol $|\ \rangle$. The kets are *not* numerical functions, just as $\boldsymbol{v}$ is not a triplet of real numbers. As in Euclidean vector algebra, the kets are defined by their formal properties.

Let $(\alpha, \beta, \ldots)$ be complex numbers and $(|\xi\rangle, |\eta\rangle, \ldots)$ be kets. By the definition of a complex vector space, the product $\alpha|\xi\rangle$ is again a vector in the space, and so is the sum

$$|\zeta\rangle = \alpha|\xi\rangle + \beta|\eta\rangle \ . \tag{13}$$

Because the scalars in the space (i.e., the 'field' over which it is defined, in mathematical parlance) are complex numbers, scalar products cannot be defined directly between pairs of kets, however. It is necessary, first, to associate a dual vector to every ket in a one-to-one manner, called a *bra*, denoted by the symbol $\langle\ |$; and second, to define the scalar products as being between bras and kets.[1] Let $\langle\xi|$ and $\langle\eta|$ be the bras dual to the indicated kets. Their scalar product is then denoted by the bra-ket $\langle\xi|\eta\rangle$, a complex number having the property

$$\langle\xi|\eta\rangle = \langle\eta|\xi\rangle^* \ , \tag{14}$$

so that the *norm* $\langle\xi|\xi\rangle$ of any ket is real, and by definition positive.[2]

In view of (14), the bra corresponding to $|\zeta\rangle$ as defined in (13) is

$$\langle\zeta| = \alpha^*\langle\xi| + \beta^*\langle\eta| \ . \tag{15}$$

Furthermore, if $|\omega\rangle$ is any ket, then the scalar product between $|\omega\rangle$ and $|\zeta\rangle$ satisfies the linear relationship

$$\langle\omega|\zeta\rangle = \alpha\langle\omega|\xi\rangle + \beta\langle\omega|\eta\rangle \ . \tag{16}$$

Ordinary Euclidean vectors satisfy the inequality $|\boldsymbol{v}\cdot\boldsymbol{w}| \leq vw$. There is a generalization of this property in $\mathfrak{H}$, the *Schwarz inequality*,

$$|\langle\xi|\eta\rangle|^2 \leq \langle\xi|\xi\rangle\langle\eta|\eta\rangle \ , \tag{17}$$

with equality being attained only if $|\xi\rangle$ and $|\eta\rangle$ are proportional to each other, or collinear. The proof of Eq. 17 is left for a problem.

A basis in $\mathfrak{H}$ is a set of kets $\{|k\rangle\}$, $k = 1, 2, \ldots$, that spans the space in the sense that any ket can be expressed as a linear combination of the basis kets. With but few exceptions, we will use orthonormal bases, that is, bases such that

$$\langle k|k'\rangle = \delta_{kk'} \ . \tag{18}$$

If $|\omega\rangle$ is an arbitrary ket, it can be expressed as a linear combination of basis kets:

$$|\omega\rangle = \sum_k \ c_k|k\rangle \ . \tag{19}$$

Because of (18),

$$c_k = \langle k|\omega\rangle \ , \tag{20}$$

and therefore

$$|\omega\rangle = \sum_k \ |k\rangle\langle k|\omega\rangle \ . \tag{21}$$

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[1] There is an analogy here to covariant and contravariant vectors in a non-Euclidean space, such as Minkowski space, where both types of vectors are needed to form Lorentz invariants.

[2] In the mathematics literature the norm is often defined as the positive square root of $\langle\xi|\xi\rangle$.

(c) Operators

This last expression gives the first hint of the power of Dirac's notation. To bring this out, consider the concept of a *subspace* of $\mathfrak{H}$, spanned by a subset of the basis vectors, and denoted by $\mathfrak{H}_S$. This subspace may be finite or infinite dimensional. Its complement $\mathfrak{H}_C$ is the remainder of $\mathfrak{H}$, so that

$$\mathfrak{H} = \mathfrak{H}_S \oplus \mathfrak{H}_C \ . \tag{22}$$

Take, in particular, the 1-dimensional subspace $\mathfrak{H}_k$ spanned by the single basis ket $|k\rangle$, and *define the projection operator* P_k *onto* $\mathcal{H}_k$ by

$$P_k|\omega\rangle = c_k|k\rangle = |k\rangle\langle k|\omega\rangle \ . \tag{23}$$

In this book we shall only indicate that an object P is an operator by the special notation $\hat{P}$ when this is not obvious from the context.

The next step is motivated by (23), namely, the introduction of what could be called an outer product between bras and kets as the definition of a *linear operator*, i.e., as an object that maps kets into linear combination of other kets (and of course bras into bras). To that end, write the right-hand side of (23) as $(|k\rangle\langle k|)|\omega\rangle$, and the projection operator as

$$P_k \equiv |k\rangle\langle k| \ . \tag{24}$$

The sum of the projection operators on *all* the basis kets is a projection on the entire space $\mathfrak{H}$, and when acting on any ket will leave it unchanged. This sum, therefore, is just the identity operator, which we simply call 1. (When it seems necessary to emphasize that it is an operator, it will be denoted by $\mathbf{1}$.) That is,

$$1 = \sum_k \ P_k = \sum_k \ |k\rangle\langle k| \ . \tag{25}$$

This is the statement that the basis spans the whole space, and is called the completeness relation. By judicious use of this form of 1, a considerable portion of what in the wave-mechanical formalism is often time and thought consuming "arithmetic" is reduced to flying by autopilot.

To see that this is so, consider

$$|\omega\rangle = 1|\omega\rangle = \left(\sum_k \ |k\rangle\langle k|\right) \cdot |\omega\rangle = \sum_k \ |k\rangle\langle k|\omega\rangle \ , \tag{26}$$

demonstrating how effortlessly Eq. 21 emerges. So does the basic identity satisfied by the projection operators on an orthonormal set:

$$P_k P_{k'} = \delta_{kk'} P_k \ , \tag{27}$$

because $P_k P_{k'} = |k\rangle\langle k|k'\rangle\langle k'|$.

Projection operators onto multi-dimensional subspaces can also be defined by generalizing (24). Let $\mathcal{K}$ designate a set of kets $|k_i\rangle, i = 1, \ldots, n$, which span the subspace $\mathfrak{H}_\mathcal{K}$. The projection operator onto this subspace is then

$$P_\mathcal{K} = \sum_{i=1}^{n} |k_i\rangle\langle k_i| \ , \qquad P_\mathcal{K}^2 = P_\mathcal{K} \ . \tag{28}$$

Let $\mathcal{K}'$ be some other subspace *orthogonal* to $\mathcal{K}$, i.e., having no basis kets in common with $\mathcal{K}$, and define $P_{\mathcal{K}'}$ as in (28). Then

$$P_{\mathcal{K}} P_{\mathcal{K}'} = 0 \ , \tag{29}$$

in obvious generalization of (27).

Next, define two operators $X = |a\rangle\langle b|$ and $Y = |c\rangle\langle d|$, where the bras and kets are arbitrary. The product of an operator with with any ket or bra are then defined by generalizing the foregoing:

$$X|\xi\rangle = (|a\rangle\langle b|)|\xi\rangle = |a\rangle\langle b|\xi\rangle \ , \tag{30}$$

$$\langle\xi|X = \langle\xi|(|a\rangle\langle b|) = \langle\xi|a\rangle\langle b| \ . \tag{31}$$

The product of X and Y is defined as

$$XY = (|a\rangle\langle b|)(|c\rangle\langle d|) = |a\rangle(\langle b|c\rangle)\langle d| \ , \tag{32}$$

i.e., the operator $|a\rangle\langle d|$ multiplied by the number $\langle b|c\rangle$, and best written *without* the parentheses as

$$XY = |a\rangle\langle b|c\rangle\langle d| \ . \tag{33}$$

Properties of operators and their representation in a particular basis now follow easily. Thus if A is a linear operator, its action on a basis ket $|k\rangle$, i.e., $A|k\rangle$, is first written as $1 \cdot A|k\rangle$, and therefore

$$A|k\rangle = \sum_{k'} |k'\rangle\langle k'|A|k\rangle \ . \tag{34}$$

The complex numbers $\langle k'|A|k\rangle$ in this linear combination of kets are called the *matrix elements* of A in the k representation. The term *matrix* is appropriate because it describes the linear combination of kets that is produced by the application of two operators in succession:

$$BA|k\rangle = \sum_{k} |k'\rangle\langle k'|B \cdot 1 \cdot A|k\rangle = \sum_{k'k''} |k'\rangle\langle k'|B|k''\rangle\langle k''|A|k\rangle \ . \tag{35}$$

This is the law for matrix multiplication:

$$\langle k|BA|k'\rangle = \sum_{k''} \langle k|B|k''\rangle\langle k''|A|k'\rangle \ . \tag{36}$$

Furthermore, any operator can be written in terms of its matrix elements by writing $A = 1 \cdot A \cdot 1$ and using Eq. 25:

$$A = \sum_{kk'} |k\rangle\langle k|A|k'\rangle\langle k'| \ . \tag{37}$$

The diagonal matrix element $\langle k|A|k\rangle$ is called the expectation value of A in $|k\rangle$, for reasons to be explained in §2.2(b).

Two numbers that are global characteristics of operators appear frequently. The first is the *trace*, defined as the sum of the diagonal matrix elements, the second is the *determinant* of the matrix elements,

$$\mathrm{Tr}\, A = \sum_{k} \langle k|A|k\rangle, \qquad \det A = \det\{\langle k|A|k'\rangle\} \ . \tag{38}$$

These numbers would be of limited value were they dependent on the basis used to define the matrix elements. That they are not will emerge shortly. A caution: the trace and determinant of many operators important in quantum mechanics do not exist because the expressions that define them fail to converge when the Hilbert space in question is infinite dimensional.

From any operator A we can construct two other operators which may, or may not, differ from A. The first is the *transpose*, the second the complex conjugate:

$$A^T = \sum_{kk'} |k\rangle\langle k'|A|k\rangle\langle k'|, \qquad A^* = \sum_{kk'} |k\rangle\langle k|A|k'\rangle^*\langle k'| \ . \tag{39}$$

When $A = A^T$, the operator is called symmetric. Transposition combined with complex conjugation produces the *Hermitian adjoint* $A^\dagger$ of A:

$$A^\dagger = (A^*)^T = \sum_{kk'} |k\rangle\langle k'|A|k\rangle^*\langle k'| \ . \tag{40}$$

If $A = A^\dagger$, it is an *Hermitian operator.* Such operators play a central role in quantum mechanics. Note that

$$\langle k|A|k'\rangle^* = \langle k'|A^\dagger|k\rangle \ . \tag{41}$$

Hence if $A|\psi\rangle = |\psi'\rangle$,

$$\langle\psi'| = \langle\psi|A^\dagger \ . \tag{42}$$

It follows from these definitions that

$$(AB)^\dagger = B^\dagger A^\dagger \ . \tag{43}$$

Hence if A and B are Hermitian, their product is only Hermitian if they commute. The *commutator* is defined as

$$[A, B] = AB - BA \ ; \tag{44}$$

if A and B are Hermitian, and the commutator is not zero, it is *anti-Hermitian*, the latter meaning an operator C with the property $C^\dagger = -C$. By the same token, the *anticommutator*, defined as

$$\{A, B\} = AB + BA \ , \tag{45}$$

is Hermitian if A and B are. Operators of any type satisfy the Jacobi identity

$$[[A, B], C] + [[C, A], B] + [[B, C], A] = 0 \ . \tag{46}$$

Any operator A can be decomposed into its Hermitian and anti-Hermitian components, A_1 and A_2:

$$A_1 = \tfrac{1}{2}(A + A^\dagger) \ , \quad A_2 = \tfrac{1}{2}(A - A^\dagger) \ . \tag{47}$$

A *positive operator* is defined by the requirement that its expectation value in any ket be real and positive. Hence any positive operator is Hermitian. If A is an arbitrary operator, then both $AA^\dagger$ and $A^\dagger A$ are positive operators, but they are only identical if A_1 commutes with A_2 because

$$AA^\dagger - A^\dagger A = 2[A_2, A_1] \ . \tag{48}$$

(d) Unitary Transformations

If an operator U satisfies

$$U^\dagger U = UU^\dagger = 1 \ , \tag{49}$$

it is said to be *unitary*. In terms of the k basis, this reads

$$\sum_{k'} \langle k|U|k'\rangle\langle k''|U|k'\rangle^* = \delta_{kk''}, \qquad \text{or} \quad \sum_{k'} U_{kk'}U^*_{k''k'} = \delta_{kk''} \ , \tag{50}$$

which is the familiar definition of a unitary matrix in the notation $U_{kk'} = \langle k|U|k'\rangle$.

Unitary operators are of great importance in quantum mechanics because they describe symmetry operations and time evolution. This is intimately connected with the fact that they describe the relationship between distinct bases in $\mathfrak{H}$. Let $|r\rangle, |r'\rangle, \ldots$ be another orthonormal basis that differs from the k basis. The relations between them are

$$|r\rangle = \sum_k |k\rangle\langle k|r\rangle, \qquad |k\rangle = \sum_r |r\rangle\langle r|k\rangle \ . \tag{51}$$

The scalar products $\langle k|r\rangle$ are often called *transformation functions* because they specify how one basis is transformed into the other. They are the elements of a unitary matrix because

$$\sum_k \langle r|k\rangle\langle k|r'\rangle = \delta_{rr'}, \qquad \sum_r \langle k|r\rangle\langle r|k'\rangle = \delta_{kk'} \ , \tag{52}$$

which has the same form as (50) with $U_{rk} = \langle r|k\rangle$.

When the bases related by a unitary transformation are denumerable, the unitary operator can be written explicitly in terms of the two sets of basis vectors. Let $|a_1\rangle \ldots |a_i\rangle \ldots$ be one basis ordered in a specific manner, and $|b_1\rangle \ldots |b_i\rangle \ldots$ be the other basis ordered so that $|a_i\rangle$ is mapped into $|b_i\rangle$; define

$$U_{ba}|a_i\rangle = |b_i\rangle \ . \tag{53}$$

Then

$$U_{ba} = \sum_i |b_i\rangle\langle a_i| \ , \tag{54}$$

and

$$U^\dagger_{ba} = U_{ab}. \tag{55}$$

Furthermore, if $\{|c_i\rangle\}$ is a third basis, then

$$U_{bc}U_{ca} = U_{ba} \ . \tag{56}$$

This known as the group property of sequential unitary transformation.

The combination of operators $UAU^\dagger$, where U is unitary, is called a *unitary transformation* of A. For any pair of operators, the trace and determinant of their product satisfy the following identities:

$$\text{Tr } AB = \text{Tr } BA, \quad \det AB = (\det A)(\det B) \ . \tag{57}$$

Hence

$$\text{Tr } UAU^\dagger = \text{Tr } A, \quad \det UAU^\dagger = \det A \ . \tag{58}$$

The latter follows from (57) and

$$|\det\, U| = 1\ , \tag{59}$$

because $\det U^\dagger = (\det U)^*$, so that

$$\det\, UAU^\dagger = (\det U)(\det A)(\det U^\dagger) = |\det U|^2 \det A = \det\, A\ . \tag{60}$$

Hence the trace and determinant of any operator are invariant under unitary transformations, or as stated earlier, under a change of basis.

The projection operator $P_\mathcal{K}$ onto a subspace $\mathfrak{H}_\mathcal{K}$, defined in (28), is also invariant under unitary transformations of the basis in $\mathfrak{H}_\mathcal{K}$. This is self-evident because $P_\mathcal{K}$ is the unit operator in $\mathfrak{H}_\mathcal{K}$.

There are many ways of expressing a unitary operator U in terms of a Hermitian operator. The most common by far is

$$U = e^{iQ} = \sum_{n=0}^{\infty} \frac{(iQ)^n}{n!}\ , \tag{61}$$

where Q is Hermitian, so that $U^\dagger = e^{-iQ}$ and $UU^\dagger = 1$. This power series arises in a multitude of situations, especially in perturbation theory and in the description of continuous symmetries. Another useful form can be

$$U = \frac{1 + iK}{1 - iK}\ , \tag{62}$$

where now K is Hermitian.

The abstract language of kets and bras can now be related to the concrete language with which we started — that of the basis functions $u_a(q)$ in configuration space, their counterparts $v_a(p)$ in momentum space, and the Fourier transform involving $\phi_p(q)$ that relates these functions. To that end, recall first Eq. 1, and introduce the arbitrary ket $|\psi\rangle$, and a complete orthonormal set $|a\rangle, |a'\rangle, \ldots$, so that

$$|\psi\rangle = \sum_a\ |a\rangle\langle a|\psi\rangle\ . \tag{63}$$

On comparing with (1), we have $c_a = \langle a|\psi\rangle$.

Next, introduce a *nondenumerable* set of kets $|q_1 \ldots q_{3N}\rangle$, where all the labels take on all values on the real interval $(\frac{1}{2}L, -\frac{1}{2}L)$, which is orthonormal in the sense that

$$\langle q_1 \ldots q_{3N}|q'_1 \ldots q'_{3N}\rangle = \delta^{3N}(q - q')\ , \tag{64}$$

and complete

$$1\ =\ \int_{-\frac{1}{2}L}^{\frac{1}{2}L} dq_1 \ldots \int_{-\frac{1}{2}L}^{\frac{1}{2}L} dq_{3N}\ |q_1 \ldots q_{3N}\rangle\langle q_1 \ldots q_{3N}|\ , \tag{65}$$

where δ^{3N} was defined in (5). Obviously, deep issues of convergence and the like are being ignored, in keeping with our rough-and-ready attitudes. That being said, the linear relation between complex functions (Eq. 1) is simply the scalar product of (63) with the bra $\langle q_1 \ldots q_{3N}|$:

$$\langle q_1 \ldots q_{3N}|\psi\rangle = \sum_a\ \langle q_1 \ldots q_{3N}|a\rangle\langle a|\psi\rangle\ . \tag{66}$$

In short, ordinary functions such as $u_a(q)$ are scalar products $\langle q|a\rangle$ in the shorthand defined in Eq. 2, and in particular

$$u_a(q_1 \dots q_{3N}) = \langle q_1 \dots q_{3N}|a\rangle \ . \tag{67}$$

The representation of these *same* relationships in momentum space follows in the same way, by means of momentum space bras and kets satisfying

$$\langle p_1 \dots p_{3N}|p'_1 \dots p'_{3N}\rangle = \delta^{3N}_{pp'} \ , \tag{68}$$

$$1 = \sum_{\{p\}} |p_1 \dots p_{3N}\rangle\langle p_1 \dots p_{3N}| \ . \tag{69}$$

Here the p's take on the discrete set of values (7), so the basis is denumerable, and Kronecker as compared to Dirac deltas appear in the orthogonality relation. Equations (11) and (12) are then simply

$$\langle p|a\rangle = \int (dq)\langle p|q\rangle q\langle a\rangle, \quad \langle q|a\rangle = \sum_p \langle q|p\rangle\langle p|a\rangle \ , \tag{70}$$

which identify the product of plane waves $\phi_p(q)$ of Eq. 8 as the elements of the unitary transformation from the q to the p basis:

$$\langle q_1 \dots q_{3N}|p_1 \dots p_{3N}\rangle = \prod_{j=1}^{3N} \frac{e^{iq_j p_j/\hbar}}{\sqrt{L}} \ . \tag{71}$$

This last expression brings out an important if rather obvious point: *the Hilbert spaces for the separate degrees of freedom are independent, and the space for the whole system is a direct product of such spaces:*

$$\mathfrak{H} = \mathfrak{H}_1 \otimes \mathfrak{H}_2 \dots \otimes \mathfrak{H}_{3N} \ . \tag{72}$$

The kets in the q and p bases are also products, e.g.,

$$|p_1 p_2 \dots p_{3N}\rangle = |p_1\rangle \otimes |p_2\rangle \dots \otimes |p_{3N}\rangle \ . \tag{73}$$

Not all kets in $\mathfrak{H}$ are of this product form, however! An arbitrary ket $|\psi\rangle$ will be such a product only if just one term appears in the sum of Eq. 1, and the function u_a is itself a product.

There is an asymmetry in the preceding definitions of the p and q bases: the former is denumerable and the latter is not. The q basis can also be made denumerable by replacing the spatial continuum $(-\frac{1}{2}L, \frac{1}{2}L)$ by a discrete lattice with a spacing much smaller than any dimension of physical interest. That is often done in numerical work, and sometimes in purely theoretical discussions. Conversely, the discrete momentum space can be replaced by a continuum by taking the limit $L \to \infty$. That we will often do. To see how, it suffices to look at just one degree of freedom, i.e., one factor in (72), and to replace the plane wave in (71) as follows:

$$\frac{e^{iqp/\hbar}}{\sqrt{L}} \longrightarrow \frac{e^{iqp/\hbar}}{\sqrt{2\pi\hbar}} \equiv \varphi_p(q) \ . \tag{74}$$

These functions are normalized to delta functions:

$$\int_{-\infty}^{\infty} dp\, \varphi_p(q)\varphi_p^*(q') = \delta(q-q'), \qquad \int_{-\infty}^{\infty} dq\, \varphi_p^*(q)\varphi_{p'}(q) = \delta(p-p') \ , \tag{75}$$

so that with these definitions the $q-p$ transformation function is

$$\langle q|p\rangle_\infty = \varphi_p(q) \ , \tag{76}$$

and

$$1 \ = \ \int_{-\infty}^{\infty} dp\, |p\rangle_\infty \langle p|, \qquad \langle p|p'\rangle_\infty = \delta(p-p') \ . \tag{77}$$

The suffix ∞ will not be shown again because it should be obvious whether the discrete or continuous basis is in use.

(e) Eigenvalues and Eigenvectors

Finally, we summarize crucial properties of Hermitian operators. The following are well-known facts about d-dimensional complex vector spaces $\mathfrak{C}_d$, provided d is finite:

1. Any *single* Hermitian operator A on $\mathfrak{C}_d$ can be diagonalized by a unitary transformation.

2. The elements of this diagonalized form are real and are called the *eigenvalues* of A, designated by $a_1, \ldots a_d$. They need not all be different; sets having the same value are called *degenerate*. The set of all eigenvalues is called the *spectrum* of A.

3. The eigenvalues are the roots of *the secular equation*

$$\det\,(A - a\mathbf{1}) = 0 \ , \tag{78}$$

   i.e., the roots of an algebraic equation of degree d.

4. The basis vectors $|1\rangle \ldots |d\rangle$ that diagonalize A are called its *eigenvectors or eigenkets,* and satisfy

$$A|n\rangle = a_n|n\rangle \ . \tag{79}$$

   Hence

$$A = \sum_n |n\rangle a_n \langle n| \ . \tag{80}$$

   This is called the *spectral decomposition* of the Hermitian operator A. If there are degeneracies, *all* eigenvectors within degenerate subspaces must be included in the sum for (80) to be valid.

5. Eigenvectors with different eigenvalues are orthogonal. Those that belong to a degenerate subspace will not be orthogonal automatically, but orthogonal linear combinations can always be built from them.

6. If A_i, where $i = 1, \ldots, K$, is a set of K *commuting* Hermitian operators, these operators can be diagonalized simultaneously, with eigenvalues $\{a_n^{(i)}\}$. The eigenvectors satisfy

$$(A_i - a_n^{(i)})|a_n^{(1)} a_n^{(2)} \ldots a_n^{(K)}\rangle = 0 \ , \tag{81}$$

where the eigenvectors are now designated by the simultaneous eigenvalues. Any two eigenvectors are orthogonal if any of their eigenvalues differ.

7. If a pair of Hermitian matrices do *not* commute, they *cannot* be diagonalized simultaneously.

8. If $|a\rangle$ is an eigenket of A with eigenvalue a, and B is any operator (in general, not Hermitian) such that

$$[A,\ B] = \lambda B\,, \qquad \text{then} \quad B|a\rangle = \text{const.}|\lambda + a\rangle\ . \tag{82}$$

It is no small matter to establish under what circumstances these statements hold in an infinite-dimensional Hilbert space $\mathfrak{H}$, especially when the space is spanned by a nondenumerable basis, as is assumed in writing Eq. 77. For example, a force law that is singular at zero separation may produce no difficulty in classical mechanics because only a subset of classical orbits can reach the singularity, whereas in quantum mechanics it may be impossible to elude the singularity. In that case some of the statements just listed are false. While bearing this in mind, we shall assume that they are correct until disaster strikes, and march into the jungle like a naive tourist.

2.2 States and Probabilities

In the phenomena to which quantum mechanics applies, only statistical data are experimentally reproducible in most, thought not all, circumstances. It is fitting, therefore, that quantum mechanics only makes statistical predictions about most, though not all, experimental outcomes.

> *It is a central claim of quantum mechanics that the statistical character of quantum mechanics is irreducible — that there are no underlying "hidden variables" which behave in a deterministic manner, and that this statistical character is not an expression of ignorance about such hidden substructure.*

Here the word "claim" is not to be read as hypothesis. At one time it was possible to leave it for the future to decide whether the existence of such hidden substructure is a plausible hypothesis, but that option only survives now in a non-local form we find unacceptable. It must be stressed that here "hidden substructure" does *not* mean further degrees of freedom that are still invisible at presently available energies, but degrees of freedom that are at work in familiar phenomena but not seen, and which supposedly account for the properties of quantum states that are perplexing from a classical perspective.[1] Hidden variable embellishments of quantum mechanics, as we shall see in chapter 12, are in conflict with experiment unless the additional variables interact instantaneously over arbitrary distances and thereby violate the relativistic principle of causality. As we learned from two-particle interferometry in §1.2, the quantum state can have both wave-like and particle-like

[1] Further *quantum* degrees of freedom, such as nucleons "inside" nuclei but ignored in atomic physics, or speculative constituents of leptons, are irrelevant to this issue.

correlations between distant non-interacting subsystems, and it has this property without violating causality, an amazing performance that classically motivated depictions cannot duplicate.

(a) Quantum States

The quantum state, as represented by the Schrödinger wave function $\Psi(\boldsymbol{r}_a \boldsymbol{r}_b)$, already appeared in our treatment of two-particle interferometry. Whether Ψ refers to an individual pair, or to an ensemble of such pairs, is a question that was not raised. Given the statistical nature of phenomena in the quantum realm, it seems natural to associate the quantum state with an ensemble of identical systems $\mathcal{S}$, with the probabilities the frequencies with which various specific properties of $\mathcal{S}$ occur. That is a widely held view, which we shared for many years, though as believers in the ensemble interpretation we were in the habit of speaking and thinking in the singular — *the* atom, *the* electron, etc.

Consider, however, the statement which closed §1.2: Ψ *must be able to display itself in a wave-like or particle-like guise, or in various combinations of these guises, depending, so to say, on what question will be asked of it in the future.* Recall, furthermore, that the EPR feature arises when the choice is made, *on an event-by-event basis and at random,* between determining the position or the momentum of one or the other particle belonging to a single pair. Thus an *individual* pair displays a richness of distinct properties which makes it rather contrived to think of the quantum state as being nothing beyond a description of an ensemble of pairs. Of course, this is not a proof that the ensemble interpretation is invalid. That said, *we will assume that the quantum state is associated with individual systems.* We should emphasize, moreover, that the predictions of observable effects are not contingent on whether one adheres to one or the other of these interpretations of the quantum state.

What then is meant by probability? In this interpretation, the quantum state of an individual system is endowed with *potentiality,* a term due to Heisenberg.[1] Potentiality has no numerical attribute; it is a primitive concept that quantum mechanics does not define, just as Euclidean geometry does not define the concept of point. Potentiality stands for the various properties that an individual system $\mathcal{S}$ has the potential for displaying in response to experimental tests, with probability being a property associated with the frequency of outcomes of tests on copies of $\mathcal{S}$.

We can now posit the three basic postulates of quantum kinematics; dynamics will be formulated in the following sections.

> **1.** *The most complete possible description of the state of any physical system $\mathcal{S}$ at any instant is provided by some particular vector $|\psi\rangle$ in the Hilbert space $\mathfrak{H}$ appropriate to the system. Every linear combination of such state vectors represents a possible physical state of $\mathcal{S}$.*

The last sentence is the *superposition principle.* If $\mathcal{S}$ is a system composed of N constituents which have no spin, and whose internal degrees of freedom cannot be excited in the energy regime of interest, then $\mathfrak{H}$ is the space defined in Eq. 72.

When $\mathcal{S}$ can be described by one vector, it is in a *pure state.* Should no single ket suffice, $\mathcal{S}$ is in a *mixed state*, or *mixture.* Introductory expositions of quantum

[1] Some authors use the term *propensity* in place of potentiality.

mechanics tend to focus almost exclusively on pure states, with the rationale that any mixed state can be expressed in terms of sets of pure states. While true, this does not do justice to the importance of mixtures.

The space $\mathfrak{H}$ specific to the system in question describes the full variety of pure states of $\mathcal{S}$. Properties that distinguish between states are needed, and this is provided by:

> **2.** *The physically meaningful entities of classical mechanics, such as momentum, energy, position and the like, are represented by Hermitian operators.*

Following Dirac, such operators will be called *observables*.[1] Observables that have no classical counterpart must also be anticipated, of course.

Let A be an observable. As it is Hermitian, it can be diagonalized and expressed by its spectral decomposition:

$$A = \sum_a |a\rangle a \langle a| \ . \tag{83}$$

Here $(a, a', \ldots)$ are the real eigenvalues of A, and $|a\rangle, \ldots$ the corresponding eigenkets.[2]

The last postulate defines how probabilities make their appearance:

> **3.** *A set of N identically prepared replicas of a system $\mathcal{S}$ described by the pure state $|\psi\rangle$, when subjected to a measurement designed to display the physical quantity represented by the observable A, will in each individual case display one of the values $(a, a', \ldots)$, and as $N \to \infty$ will do so with the probabilities $p_\psi(a), p_\psi(a'), \ldots$, where*
>
> $$p_\psi(a) = |\langle a|\psi\rangle|^2 \ . \tag{84}$$

This is the definition of probability in terms of the frequency of specific outcomes in a sequence of identical tests on copies of $\mathcal{S}$.

Eq. 84 is a consistent definition of a probability distribution: the real positive numbers $|\langle a|\psi\rangle|^2$ obey the sum rule

$$\sum_a \ |\langle a|\psi\rangle|^2 = \langle\psi|\psi\rangle = 1 \ , \tag{85}$$

where by convention all kets have unit norm; that is,

$$p_\psi(a) \geq 0, \qquad \sum_a \ p_\psi(a) = 1 \ . \tag{86}$$

---

[1] Dirac also used the terms c-number for ordinary numbers (in allusion to classical quantities), though possibly complex, and q-numbers for operators. Though not much used today, we sometimes return to this usage.

[2] As written, (83) refers to a discrete spectrum; should the spectrum be partially or wholly continuous, the sum is to be understood as including the appropriate integral, and some Kronecker deltas may be Dirac delta functions. This is a trivial complication at the formal level of this discussion, and will be ignored by writing all formulas as if the spectra in question are discrete.

The mean value $\langle A\rangle_\psi$ of the measurement results on a set of replicas of $\mathcal{S}$ in the state $|\psi\rangle$ is, by definition,

$$\langle A\rangle_\psi = \sum_a a\, p_\psi(a)\ , \tag{87}$$

which is the following diagonal matrix element of the observable A:

$$\langle\psi|A|\psi\rangle = \sum_a a|\langle a|\psi\rangle|^2\ . \tag{88}$$

Such mean values are called *expectation values* in quantum mechanics. Should $|\psi\rangle$ actually be the eigenket $|a\rangle$, then

$$\langle a|A|a\rangle = a\ . \tag{89}$$

Note well that (87) implies that *the only values that an observable can display are its eigenvalues.*

The probability $p_\psi(a)$ can also be expressed as an expectation value, and in that form it generalizes readily to mixed states. This is so because $p = \langle\psi|a\rangle\langle a|\psi\rangle$, whence

$$p_\psi(a) = \langle\psi|P_a|\psi\rangle\ , \tag{90}$$

where $P_a = |a\rangle\langle a|$ is the projection operator onto $|a\rangle$.

In (87) the state $|\psi\rangle$ is arbitrary. Should $|\psi\rangle$ actually be one of the eigenkets of A, say $|a_0\rangle$, the distribution is sharp, $p_{a_0}(a) = \delta_{a_0 a}$, i.e., there is no dispersion in the values displayed when the state is one of the eigenstates of A; in this case the state is guaranteed to always display one particular eigenvalue.

Thus far the probabilities associated with a pure state $|\psi\rangle$ have been expressed in terms of the eigenvalues of an observable — presumably an observable having a useful physical significance. But the definition (84) generalizes as follows. Let $|\phi\rangle$ be an arbitrary state, which together with $|\phi'\rangle, |\phi''\rangle, \ldots$ forms a complete orthonormal set, but which may not diagonalize any operator that has a useful physical significance. Then by the argument that led to (86), *the probability that a system $\mathcal{S}$ in the state $|\psi\rangle$ will be found to be in the arbitrary state $|\phi\rangle$ is*

$$p_\psi(\phi) = |\langle\phi|\psi\rangle|^2\ . \tag{91}$$

For this reason, the scalar product between states is called a *probability amplitude.*

It is natural to take it for granted that a particular value a displayed by a particular measurement of an observable A simply reveals a pre-existing value possessed by that individual specimen $\mathcal{S}$, just as your head has a definite circumference before the tape measure is unfurled in a statistical study of the egos of physicists. This entirely sensible supposition is not valid, however:

> *Values cannot be ascribed to observables prior to measurement; such values are only the outcomes of measurement.*

The common-sense inference that measurements reveal pre-existing values leads to implications that are contradicted by experiment, and are also incompatible with the Hilbert space structure of quantum mechanics. This conclusion is not obvious, and was not established firmly until some three decades after the discovery of quantum mechanics. The reasoning and experiments that lead to it will be given in

chapter 12, but the conclusion is stated here to abort seductive misconceptions. One further point should, however, be made here. Because observables have no values prior to measurement, in the ensemble interpretation of the state it is illegitimate to distinguish between the ensemble's members, for doing so would be tantamount to introducing hidden variables. This can be taken as another motivation for defining the quantum state to be a description of an individual system as compared to an ensemble.

(b) Measurement Outcomes

From what has just been said, it is clear that measurement plays a central role in relating the mathematical formalism to observable facts. If quantum mechanics purports to be a complete description of physical phenomena, it had better also describe the measurement process itself. It turns out, however, that the quantum theory of measurement is far from straightforward. For that reason we also postpone its discussion to chapter 12. Until then we take a lowbrow approach, and offer the following example as a general purpose measurement paradigm.

Let $|\psi\rangle$ be the state of a photon of a particular frequency emitted in the direction $\boldsymbol{k}$ from an atom that is in a magnetic field pointing along $\boldsymbol{n}$. Imagine a measurement apparatus $\mathcal{M}_{\text{circ}}$ that deflects any such photon into one of two directions $\boldsymbol{q}_{R,L}$ depending on whether its circular polarization is right or left-handed, and two photomultipliers that determine which of the two deflections a particular photon experienced. For arbitrary directions $\boldsymbol{k}$ and $\boldsymbol{n}$, it is impossible to predict what the next photon does, all that can be predicted is the probability for one as compared to the other deflection.

The application of the rule (91) is then as follows. Let $|\boldsymbol{k}_{R,L}\rangle$ be the states of a right- or left-circularly polarized photon propagating in the direction $\boldsymbol{k}$. Then $|\langle \boldsymbol{k}_{R,L}|\psi\rangle|^2$ are the probabilities that individual photons will be deflected in the directions $\boldsymbol{q}_{R,L}$. But any number of other questions can be addressed to $|\psi\rangle$. For example, the apparatus $\mathcal{M}_{\text{circ}}$ can be replaced by another, $\mathcal{M}_{\text{lin}}$, that measures linear polarization along two orthogonal directions $\boldsymbol{u}_{1,2}$. If $|\boldsymbol{k}_{1,2}\rangle$ are photon states with these polarizations, the corresponding probabilities are $|\langle \boldsymbol{k}_{1,2}|\psi\rangle|^2$.

Thus Eq. 91 for the probability takes for granted the existence in principle of an apparatus $\mathcal{M}_\phi$ that is able, when presented with a system $\mathcal{S}$ in the state $|\psi\rangle$, to assign it to the category that is in the state $|\phi\rangle$.

In general, a system will have several observables that all commute with each other; such observables are said to be *compatible.* It suffices to consider the case of two, A and B. There then exist simultaneous eigenkets $\{|ab\rangle\}$ of A and B with eigenvalues $(a, a', \ldots; b, b', \ldots)$. Let $f(x, y)$ be a function of two variables. Because A and B commute, the action of $f(A, B)$ on the simultaneous eigenkets is then

$$f(A, B)|ab\rangle = f(a, b)|ab\rangle \ . \tag{92}$$

Hence the expectation value of the operator f is

$$\langle\psi|f(A, B)|\psi\rangle = \sum_{ab} f(a, b)|\langle ab|\psi\rangle|^2 \ , \tag{93}$$

and by the preceding argument

$$p_\psi(ab) = |\langle ab|\psi\rangle|^2 \tag{94}$$

is the *joint probability distribution* that the observables A *and* B will display the two values a *and* b.

Note that $|\langle ab|\psi\rangle|^2$ *is not a conditional probability,* i.e., it is not the probability for the occurrence of b given that a has definitely occurred. Rather, it gives the probabilities for the occurrence of both a and b, conditional only on the state being $|\psi\rangle$. The conditional probability for b given a is

$$p_\psi(a|b) = \frac{p_\psi(ab)}{p_\psi(a)} \ . \tag{95}$$

Its distinction from the joint distribution $p_\psi(ab)$ is underscored by the identities

$$\sum_b p_\psi(a|b) = 1, \qquad \sum_b p_\psi(ab) = p_\psi(a) \ . \tag{96}$$

The most famous and familiar example of what has just been said is provided by the Schrödinger wave function. In Dirac's language it is the scalar product of $|\psi\rangle$ with a simultaneous eigenket $|q_1 \dots q_{3N}\rangle$ of all the coordinate operators,

$$\psi(q_1 \dots q_{3N}) \equiv \langle q_1 \dots q_{3N}|\psi\rangle \ . \tag{97}$$

The *Born interpretation* of $|\psi(q_1 \dots q_{3N})|^2$ as a joint probability distribution of the coordinates in an N-particle state is a special case of the meaning ascribed to scalar products quite generally.

Now to a situation that has no classical counterpart, the case of *incompatible observables, i.e., observables that do not commute*. Call such a pair P and Q, where these names are merely suggestive; they need not be momentum or coordinate. There are then eigenkets of P and Q, satisfying

$$P|p\rangle = p|p\rangle, \qquad Q|q\rangle = q|q\rangle \ , \tag{98}$$

but simultaneous eigenkets of P *and* Q *do not exist*. While probability distributions for the eigenvalues of P *or* of Q are of the same form as before, namely

$$p_\psi(p) = |\langle p|\psi\rangle|^2, \qquad p_\psi(q) = |\langle q|\psi\rangle|^2 \ , \tag{99}$$

it is not possible to define a joint distribution for the two eigenvalue sets $\{p\}$ and $\{q\}$.

To see why, try the following: calculate the probability that $|\psi\rangle$ will display a particular eigenvalue p of P, then the probability that this eigenstate of P will display the eigenvalue q of Q, and sum over *all* values of p in the expectation that this will give the probability $p_\psi(q)$ that $|\psi\rangle$ will display the value q when there is no knowledge about p. That is, form

$$\sum_p p_p(q)p_\psi(p) = \sum_p \left[|\langle q|p\rangle|^2 \times |\langle p|\psi\rangle|^2\right] \ . \tag{100}$$

Compare this to

$$p_\psi(q) = |\langle q|\psi\rangle|^2 = \Big|\sum_p \langle q|p\rangle\langle p|\psi\rangle\Big|^2 \ . \tag{101}$$

The naive, or classical, way of composing probabilities (Eq. 100) disagrees with that of quantum mechanics (Eq. 101). In the latter the two probability amplitudes

for $\psi \to p$ and $p \to q$ — both complex numbers — are *first* multiplied, *then* summed over the intermediate variable p, and it is the absolute square of this sum that gives the probability for q in the state $|\psi\rangle$, — a far cry from "common-sense" multiplication of probabilities! When the probabilities are combined as in (100), the phases of the probability amplitudes do not matter, whereas in the *coherent superposition* (101) these phases are crucial.

What is the reason for this striking difference? It is not that the familiar composition law of Eq. 100 is wrong, but that it corresponds to a sequence of measurements that differs from the one that determines $p_\psi(q)$.

In the situation summarized by (100), there is first a measurement apparatus $\mathcal{M}_P$ that assigns each specimen in the state $|\psi\rangle$ to the set that possess the eigenvalue p of P, as a consequence of which these individuals are *known* to be in the state $|p\rangle$; subsequently, each system that is in the state $|p\rangle$ is passed into a second apparatus $\mathcal{M}_Q$ which is able to ask "do you belong in $|q\rangle$," with the answer being "perhaps, with probability $|\langle q|p\rangle|^2$." The first segregation produces a set with the property p having the fractional population $p_\psi(p)$, so that the fraction of the systems that were in $|\psi\rangle$ that survive both filtrations is $p_p(q)p_\psi(p)$. The sum on p in (100) only results in a *recoverable* loss of knowledge, as in a demographic study that sums over cities when stating what fraction of a country's urban population ponders the meaning of quantum mechanics. That is to say, the same result $\sum_p p_p(q)p_\psi(p)$ is found by discarding all but one of the sets produced by $\mathcal{M}_P$ in the first measurement, then using this set of individuals as the input for $\mathcal{M}_Q$, and repeating this experiment for all the other sets produced by $\mathcal{M}_P$. The resemblance to demography is very poor, of course: as P and Q are incompatible, the second measurement $\mathcal{M}_Q$ produces individuals $|q\rangle$ which no longer have a definite value of p. This is confirmed by passing a set of outputs $|q\rangle$ from $\mathcal{M}_Q$ through the device $\mathcal{M}_P$, because the latter will have as its output sets $|p\rangle$ with a variety of values p.

The measurement that gives the result (101) is one in which a system in the state $|\psi\rangle$ is sent directly to $\mathcal{M}_Q$; the states $|p\rangle$ that appear in this equation are in essence a mathematical artifact, for any complete set gives the same result. The probability $p_\psi(q)$ determined in this way cannot be diagnosed or dissected to find $p_p(\psi)$. In contrast, if some other complete set $|a\rangle$ is used in (100), it will give a different result.

To summarize, both probability calculations make perfectly good sense, but they correspond to very different physical processes if P and Q are incompatible observables.

A final point must still be made about pure states. Probabilities involve only the *absolute values* of scalar products between vectors in a Hilbert space, while expectation values are *bilinear* in them. Therefore, replacing any ket $|\psi\rangle$ by $e^{i\alpha}|\psi\rangle$, where α is real, does not alter expectation values or probabilities. Thus it is not really correct to say that pure physical states corresponds to a single ket in a Hilbert space. Rather, the set of kets $e^{i\alpha}|\psi\rangle$ describes one physical state. Such a set is called a ray, and therefore *the state space of quantum mechanics is really a ray space, not a Hilbert space.*

It therefore seems unjustified to require various statements in quantum mechanics to be invariant under unitary transformations, because it is not relations between kets but between rays that have physical significance. Thanks to a theorem by Wigner (§7.1), this headache rarely arises, because the theorem proves that the

only physically significant transformations that cannot be represented by unitary transformations on kets is time reversal.

(c) Mixtures and the Density Matrix

Although pure states abound in text books and research papers, systems in the real world are rarely in pure states. For example, the beam produced by an accelerator is hardly a coherent superposition of momentum eigenstates, as it would have to be if it were to be represented by a pure state. A more common example is that of a collection of atoms in thermodynamic equilibrium.

Consider the latter. Here the key observable is the Hamiltonian H with energy eigenvalues $\{E\}$. There will, in general, be other observables compatible with H, e.g., angular momentum, designated collectively by A, that together specify a basis $\{|Ea\rangle\}$ in $\mathfrak{H}$. At temperature T these states are populated in accordance with the Boltzmann probability distribution,

$$p_T(E) = e^{-E/kT}/Z \ , \tag{102}$$

where k is Boltzmann's constant and Z a normalization factor called the partition function. Requiring the probabilities to sum to one then fixes Z:

$$Z = \sum_{E,a} e^{-E/kT} \ . \tag{103}$$

In this and similar sums, all states belonging to a given energy eigenvalue must be included.

The expectation value of some observable Q, which need not be compatible with the the Hamiltonian, is then its expectation value in the various states $|Ea\rangle$ weighted by the thermal probability distribution,

$$\langle Q\rangle_T = \sum_{E,a} p_T(E)\, \langle Ea|Q|Ea\rangle \ . \tag{104}$$

This expectation value is thus the result of two very different averages: that due to the statistical distribution of eigenvalues of Q in the pure states $|Ea\rangle$, and that due to the probability that such a pure state occurs in the thermal ensemble:

$$\langle Q\rangle_T = \sum_{E,a} \sum_{q} q\, p_T(E)\, |\langle q|Ea\rangle|^2 \ . \tag{105}$$

By introducing an operator ρ called the *density matrix*, expectation values such as $\langle Q\rangle_T$ can be written in a form that at first sight is opaque but which turns out to be very powerful.[1] The nomenclature "matrix" is somewhat unfortunate, because ρ is an operator, and many authors call it the statistical or density operator. But the more common usage is so long established that, as with many other terms in physics, it is best to accept it as an indelible part of our cultural heritage, and to not balk at phrases like "the matrix elements of the density matrix are ...."

[1] The density matrix was introduced by Landau and developed into its prominent role by von Neumann.

The density matrix describing a thermal equilibrium ensemble is defined as

$$\rho_T = \sum_{E,a} |Ea\rangle p_T(E) \langle Ea| = \sum_{E,a} p_T(E)\, P_{Ea} \ , \tag{106}$$

i.e., a sum of projection operators onto the basis $\{|Ea\rangle\}$ weighted by the Boltzmann distribution. Because the probabilities $p_T(E)$ are normalized to 1,

$$\mathrm{Tr}\, \rho_T = 1 \ . \tag{107}$$

In terms of ρ_T, the expectation value of Q then has the compact and very useful form

$$\langle Q \rangle_T = \mathrm{Tr}\, \rho_T Q \ ; \tag{108}$$

This formulation allows us to give a basis-independent distinction between pure states and mixtures. Again, let $|\psi\rangle$ be some pure state, and

$$P_\psi = |\psi\rangle\langle\psi| \tag{109}$$

its associated projection operator. Then the expectation value in the pure state $|\psi\rangle$ is

$$\langle\psi|Q|\psi\rangle = \sum_{a,a'} \langle a|\psi\rangle\langle\psi|a'\rangle\langle a'|Q|a\rangle = \mathrm{Tr}\, P_\psi Q \equiv \mathrm{Tr}\, \rho_\psi Q \ . \tag{110}$$

That is to say, *in the case of a pure state, the density matrix is a projection operator onto the state.* Consequently, the density matrix of a pure state is characterized by

$$(\rho_\psi)^2 = \rho_\psi \ , \qquad \mathrm{Tr}\ (\rho_\psi)^2 = 1 \ . \tag{111}$$

The latter, as promised, is a statement that does not depend on the basis because the trace is invariant under unitary transformations.

Consider now the square of the thermal density matrix (Eq. 106):

$$(\rho_T)^2 = \sum_{E,a} [p_T(E)]^2 P_{Ea} \ . \tag{112}$$

Hence

$$\mathrm{Tr}\ (\rho_T)^2 = \sum_{E,a} [p_T(E)]^2 < 1 \ . \tag{113}$$

The sum is only one if the temperature is strictly zero, so that only the ground state is occupied, i.e., the case of a pure state.

The example of the thermal distribution is illustrative, but holds for any set of probabilities. The general situation is summarized as follows:

> *A state is pure if its density matrix ρ is a projection operator, and it is a mixture if it is not. The two cases are characterized by the invariant condition*
>
> $$\mathrm{Tr}\, \rho^2 \leq 1 \ , \tag{114}$$
>
> *with the equality only holding if the state is pure.*

Thus far the density matrix has been written in terms of projection operators. Like all operators, it can be written in any basis, and defined without reference to a particular basis — namely, as an observable whose eigenvalues $(p_1, p_2, \ldots)$ satisfy

$$0 \leq p_i \leq 1, \qquad \sum_i p_i = 1 \ . \tag{115}$$

The state is pure if, and only if, all eigenvalues p_i of ρ but one vanish.

Let $|a_i\rangle$ be the orthonormal basis that diagonalizes ρ, so that

$$\rho = \sum_i |a_i\rangle p_i \langle a_i| \ . \tag{116}$$

The expectation value of an observable Q is then given by (104),

$$\langle Q \rangle = \sum_i p_i \langle a_i|Q|a_i\rangle \ . \tag{117}$$

in general, therefore, the expectation value of an observable Q in a state ρ, whether pure or mixed, can be written in the invariant form

$$\langle Q \rangle = \mathrm{Tr}\, \rho\, Q \ . \tag{118}$$

The expression that gives the probability of a finding a state $|\phi\rangle$ in a pure state (Eq. 90) can be extended to the case of a mixture, namely,

$$p_\phi(\rho) = \mathrm{Tr}\, \rho\, P_\phi = \langle \phi|\rho|\phi\rangle \, . \tag{119}$$

In terms of the basis of (116), this reads

$$p_\phi(\rho) = \sum_i p_i |\langle \phi|a_i\rangle|^2 \ , \tag{120}$$

as it must.

The most important measure of the departure from purity is provided by *the von Neumann entropy* S. For any state ρ, it is defined as

$$S = -k\, \mathrm{Tr}\, \rho\, \ln \rho \ , \tag{121}$$

where k is Boltzmann's constant. When ρ is the Boltzmann distribution, S is the entropy of statistical thermodynamics (see Prob. 3); in terms of the probabilities p_i it has the familiar form

$$S = -k \sum_i p_i \, \ln p_i \ . \tag{122}$$

For a pure state, where only one $p_i = 1$ and the others vanish, $S = 0$. Furthermore $S \geq 0$ because $0 \leq p_i \leq 1$. This leads to the question of whether S has a maximum value. To answer this, one varies the probabilities in S under the constraint that they sum to 1. This is done by introducing a Lagrange multiplier λ,

$$\delta \sum_i p_i \, (\ln p_i + \lambda) = 0 \ , \tag{123}$$

or

$$\sum_i \delta p_i \,(\ln p_i + 1 + \lambda) = 0 \ . \tag{124}$$

The variations δp_i in (124) are now independent, and therefore $\ln p_i + 1 + \lambda = 0$, i.e., the p_i that maximize S do not depend on i. But they must sum to 1, hence this whole argument only makes sense as it stands if the Hilbert space $\mathfrak{H}_d$ has a finite dimension d, so that $p_i = 1/d$.

The entropy therefore satisfies the inequalities

$$0 \le S \le k \ \ln d \ , \tag{125}$$

and the density matrix that maximizes S is

$$\rho_{\max} = \frac{1}{d} \sum_i |a_i\rangle\langle a_i| \ . \tag{126}$$

At first sight, $\{|a_i\rangle\}$ is a particular basis that diagonalizes ρ. But the sum in (126) is just the unit operator, so

$$\rho_{\max} = \frac{1}{d} \ . \tag{127}$$

In short, the mixture in which the entropy is maximal is the one in which all states, in any basis, are populated with equal probability. Put another way, $S = 0$ when there is maximal knowledge in that the state is pure, and $S = S_{\max}$ when the available states are populated at random.

We must still address the following basic question: *Given an unlimited set of replicas of a system $\mathcal{S}$ in an unknown state ρ, known to reside in a d-dimensional Hilbert space $\mathfrak{H}_d$, what measurements must be carried out to determine this state?* The unknown density matrix (whether pure or mixed) is a d-dimensional Hermitian matrix of unit trace is specified by $d^2 - 1$ real parameters. According to Eq. 37 and Eq. 41, in terms of an the arbitrary basis $\{|a_i\rangle\}$ in $\mathfrak{H}_d$, the operator ρ has the form

$$\rho = \sum_{ij} |a_i\rangle r_{ij} \langle a_j| \ , \qquad r_{ij} = r^*_{ji} \ . \tag{128}$$

An arbitrary observable in $\mathfrak{H}_d$ is a linear combination, with real coefficients, of the d^2 Hermitian operators

$$X_{ij} = \tfrac{1}{2}\{|a_i\rangle\langle a_j| + |a_j\rangle\langle a_i|\} \ , \quad Y_{ij} = \tfrac{1}{2} i\{|a_i\rangle\langle a_j| - |a_j\rangle\langle a_i|\} \ . \tag{129}$$

Of these, the combination $\sum_i X_{ii} = 1$ is trivial. Because $\mathrm{Tr}\,\rho\,|a_i\rangle\langle a_j| = r_{ji}$,

$$\mathrm{Tr}\,\rho\, X_{ij} = \mathrm{Re}\, r_{ij} \ , \quad \mathrm{Tr}\,\rho\, Y_{ij} = \mathrm{Im}\, r_{ij} \ . \tag{130}$$

In consequence, when faced with an arbitrary unknown state in $\mathfrak{H}_d$, to identify the state unambiguously the expectation values of a complete set of observables must be measured, where by 'complete' is meant a set that allows the evaluation of all the (d^2-1) nontrivial expectation values appearing in (130). A concrete example should help to make this inscrutable enumeration understandable. Take the case where $\mathcal{S}$ is an atom with angular momentum 1, whose states live in a 3-dimensional Hilbert space. According to what has just been learned, the expectation values of eight observables must be measured. As shown in §3.3, they are the three independent components of the atom's magnetic moment vector and the five independent components of its quadrupole tensor (a Cartesian tensor of rank 2).

(d) Entangled States

There is a common and serious misconception that mixtures only arise when pure states are "mixed" by the environment, such as a temperature bath, or by some apparatus, such as an accelerator. Not so: *If a composite system is in a pure state, its subsystems are in general in mixed states.* This is the context in which mixtures are often important in discussions of the interpretation of quantum mechanics, and also in many other contexts.

To see how mixtures arise from pure states, consider a system composed of two subsystems with coordinates q_1 and q_2. Let $|\Psi\rangle$ be an arbitrary pure state of the system, with wave function $\Psi(q_1 q_2)$, so that its density matrix is

$$\langle q_1 q_2|\rho|q_1' q_2'\rangle = \Psi(q_1 q_2)\Psi^*(q_1' q_2') \ . \tag{131}$$

Let A_1 be an observable of the subsystem 1; that is, insofar as subsystem 2 is concerned it is the unit operator:

$$\langle q_1 q_2|A_1|q_1' q_2'\rangle = \langle q_1|A_1|q_1'\rangle\, \delta(q_2 - q_2') \ , \tag{132}$$

where, to make contact with the wave-function language clearer the spectra are taken to be continuous. Hence the expectation value of A_1 in Ψ is

$$\langle A_1\rangle_\Psi = \int dq_1\, dq_1'\, dq_2\ \Psi^*(q_1 q_2)\langle q_1|A_1|q_1'\rangle\Psi(q_1' q_2) \ . \tag{133}$$

This expectation value can be written in terms of a *reduced density matrix* ρ_1 describing only the first subsystem, and defined as

$$\langle q_1|\rho_1|q_1'\rangle = \int dq_2\ \langle q_1 q_2|\Psi\rangle\langle\Psi|q_1' q_2\rangle \ = \int dq_2\ \langle q_1 q_2|\rho|q_1' q_2\rangle \ . \tag{134}$$

Then Eq. 133 is

$$\langle A_1\rangle_\Psi = \int dq_1\, dq_1'\ \langle q_1|A_1|q_1'\rangle\langle q_1'|\rho_1|q_1\rangle = \mathrm{Tr}\, A_1\rho_1 \ . \tag{135}$$

That is to say, for all expectation values pertaining only to subsystem 1, the density matrix *is* ρ_1.

We will now show that *a subsystem is not in a pure state when the whole system that contains it is in a pure state* Ψ *unless* Ψ *has the form of a product.* In terms of our example, consider

$$\Psi(q_1 q_2) = c_1 u_1(q_1)v_1(q_2) + c_2 u_2(q_1)v_2(q_2)\,, \quad |c_1|^2 + |c_2|^2 = 1 \tag{136}$$

where u_i and v_j are orthonormal,

$$\int dq_1\, u_i^*(q_1)u_j(q_1) = \delta_{ij}, \qquad \int dq_2\, v_i^*(q_2)v_j(q_2) = \delta_{ij} \ . \tag{137}$$

When neither coefficient in (136) vanishes, Ψ is called an *entangled state,*[1] i.e., one that *cannot* be written as a simple product

$$\Psi(q_1 q_2) = \varphi(q_1)\chi(q_2) \ . \tag{138}$$

[1] Entangled states first appeared in Heisenberg's theory of He (see §6.2), but their full significance was first recognized by Schrödinger, and the term is due to him.

That (136) cannot be written in the form (138) will now be proven.

Thanks to (137), it follows from (136) that

$$\langle q_1|\rho_1|q_1'\rangle = |c_1|^2 u_1(q_1)u_1^*(q_1') + |c_2|^2 u_2(q_1)u_2^*(q_1') \ , \tag{139}$$

i.e., a density matrix for system 1 with probabilities $|c_i|^2$ for being in the state with wave function $u_i(q_1)$. That ρ_1 does not describe a pure state of *subsystem 1* is clear, because

$$\langle q_1|(\rho_1)^2|q_1'\rangle = |c_1|^4 u_1(q_1)u_1^*(q_1') + |c_2|^4 u_1(q_1)u_1^*(q_1') \ , \tag{140}$$

so that

$$\text{Tr } (\rho_1)^2 = |c_1|^4 + |c_2|^4 < 1 \ . \tag{141}$$

Thus ρ_1 is not pure, and therefore cannot be represented by any single state in the Hilbert space of system 1, unless one of the coefficients $c_{1,2}$ vanishes, in which case Ψ has the product form, i.e., is not entangled, *QED.*

This result generalizes to composites of more than two subsystems and to more complicated states than Eq. 136. Namely, the density matrix of a subsystem ρ_s can only be that of a pure state if the density matrix ρ of the whole system is of the form $\rho_s \otimes \rho_R$, where ρ_s is itself pure and ρ_R is the density matrix of the remainder. If ρ has this product form all joint distributions will be products with one factor pertaining to the subsystem s and the other factor pertaining to the remainder.

Entangled states have correlations which are very weird from any classical perspective. This property is of crucial importance in such disparate topics as the spectrum of He and magnetism (§6.2), and in Bell's theorem (§12.3). The two-body probability distribution associated with the state (136) is

$$p(q_1q_2) = |c_1|^2|u_1(q_1)|^2|v_1(q_2)|^2 + |c_2|^2|u_2(q_1)|^2|v_2(q_2)|^2 + I_2(q_1q_2) \ , \tag{142}$$

$$I_2(q_1q_2) = 2\,\text{Re}\,\{c_1c_2^*\,u_1(q_1)u_2^*(q_1)v_1(q_2)v_2^*(q_2)\} \ . \tag{143}$$

The first two terms are mundane, but the interference term I_2 is very strange. For example, if the wave functions u_i and v_i are free particle wave packets describing particles that are running off to large distances in various directions, the interference term describes correlations even though the particles do not interact and are far apart.

The strange two-body interference term I_2 does not survive in the probability distribution for one subsystem, e.g., in $\langle q_1|\rho_1|q_1\rangle$, but this is only the case when the entangled state is composed of orthogonal wave functions. And even when they are orthogonal, the two-body interference term is crucial in situations such as those just mentioned.

Finally, we ask how and whether two pure states can be distinguished. For this purpose, consider a pure entangled state for a two-body system (a, b) of the type provided by the interferometer in §1.2:

$$\Phi(q_aq_b) = N[\varphi_1(q_a)\chi_1(q_b) + \varphi_2(q_a)\chi_2(q_b)] \ . \tag{144}$$

Here φ_n and χ_n are arbitrary wave functions for a and b, respectively, which in general are *not* orthogonal; N is the normalization factor. The probability distribution associated with Φ has the two-body interference term

$$I_2(q_aq_b) = 2N^2\text{Re}\,\{\varphi_1(q_a)\varphi_2^*(q_a)\chi_1(q_b)\chi_2^*(q_b)\} \ . \tag{145}$$

The correlations between a and b when they are widely separated are contained in I_2. If, however, no measurement whatever is performed on b, the probability distribution for a is that of a mixture, with the one-body interference term

$$I_1(q_a) = 2N^2 \mathrm{Re}\,\{V\varphi_1(q_a)\varphi_2^*(q_a)\}\ , \tag{146}$$

where

$$V = \int dq_b\, \chi_1(q_b)\chi_2^*(q_b)\ . \tag{147}$$

Hence a by itself will only show an interference pattern if the states $\chi_{1,2}$ of the other body b are *not* orthogonal. This last statement is illustrated by the interferometer of §1.2: the two states of b that arrive at the detector D_b are orthogonal because they have differing momenta along the y direction, so in accordance with the preceding statement a does not display an interference pattern.

A somewhat different experimental setup than the one of §1.2 will elucidate the condition required for V not to vanish (see Fig. 2.1). Assume that the particles a

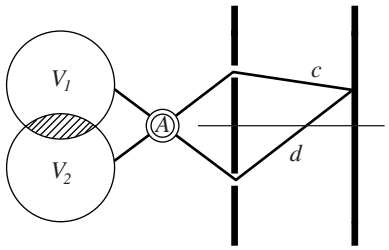

FIG. 2.1. A modification of the two particle interferometer of §1.2, in which the parent A decays into charged daughters (e.g., $K^0 \to \pi^+ + \pi^-$), with one decay product captured into somewhat overlapping traps on the left, while the other passes through one of two holes on the right on its way to the detector.

and b are charged, as in the decay $K \to \pi^+ + \pi^-$, and that the interferometer is replaced by an apparatus in which the left-hand screen and detector are replaced by magnetic traps that capture b into one of the states $\chi_{1,2}(q_b)$ when a has passed through either the upper or lower right-hand hole. Then a will show an interference pattern provided there is a spatial overlap between the two trapped states of b, i.e., provided they are *not* orthogonal. The significance of this overlap can be stated in two, at first sight quite different, ways: (i) on the mathematical side, that the states of b are not orthogonal; (ii) on the physical side, that the states of b do not unambiguously determine the path of a.

The general lesson to be drawn from these examples is that a pair of states, if they are orthogonal, can give a yes-no answer as to whether an observable has a particular value, whereas the answer becomes increasingly ambiguous as their overlap increases. For that reason, the *visibility* $|V|^2$ *of the interference pattern displayed by* a *alone is a measure of the confidence with which an observation on* b *determines the state of* a.

(e) The Wigner Distribution

Quantum states, whether pure or mixed, can be cast into a form that is astonishingly reminiscent of phase space distributions in classical statistical mechanics.

Consider a one-dimensional system with density matrix $\langle q|\rho|q'\rangle$ in the coordinate representation; the generalization to more degrees of freedom is trivial and will be stated at the end. *The Wigner distribution* is then defined by

$$f(q,p) = \int_{-\infty}^{\infty} ds\, e^{-ips/\hbar}\, \langle q + \tfrac{1}{2}s|\rho|q - \tfrac{1}{2}s\rangle \ . \tag{148}$$

Wigner's function $f(q,p)$ has three properties that coincide with those of a classical phase space distribution. First, as ρ is Hermitian, f is real. Second, integration of f over momentum gives the probability distribution of the coordinate:

$$\int \frac{dp}{2\pi\hbar}\, f(q,p) = \langle q|\rho|q\rangle \ . \tag{149}$$

And third, integration over the coordinate gives the probability distribution of the momentum:

$$\int \frac{dq}{2\pi\hbar}\, f(q,p) = \langle p|\rho|p\rangle \ . \tag{150}$$

Despite these marvelous properties, $f(q,p)$ is *not* a probability distribution because it is not positive definite for arbitrary states. This is hardly astonishing because the incompatibility of coordinate and momentum, or put equivalently, the uncertainty principle, implies that joint probability distributions of q and p cannot exist except under special circumstances. For example, as we will learn in §4.2, the ground state is the only energy eigenstate of the harmonic oscillator that has a positive definite Wigner distribution.

Observables can also be cast into a form due to Weyl that give them the appearance of functions in phase space. Let A be any observable, and define a function $\mathcal{A}(q,p)$ by requiring that it produce the correct expectation value when averaged over the Wigner distribution:

$$\int \frac{dq\,dp}{2\pi\hbar}\, \mathcal{A}(q,p)\, f(q,p) = \mathrm{Tr}\ A\rho \ . \tag{151}$$

It is left to the reader to show that $\mathcal{A}$ has precisely the same relationship to A as does f to ρ:

$$\mathcal{A}(q,p) = \int ds\, e^{-ips/\hbar}\, \langle q + \tfrac{1}{2}s|A|q - \tfrac{1}{2}s\rangle \ . \tag{152}$$

Two important special cases are observables which are diagonal in the coordinate or momentum representation, such as a potential V or a kinetic energy K, respectively. That is, define

$$\langle q|V|q'\rangle = \delta(q-q')\, V(q) \ , \qquad \langle p|K|p'\rangle = \delta(p-p')\, K(p) \ . \tag{153}$$

Then, according to (152), their "phase space" counterparts are

$$\mathcal{V}(q,p) = V(q) \ , \qquad \mathcal{K}(q,p) = K(p) \ . \tag{154}$$

This, of course, is required by (149) and (150).

The generalization to a N particles is simply

$$dq \to dq_1 \ldots dq_{3N} \ , \qquad \frac{dp}{2\pi\hbar} \to \frac{dp_1}{2\pi\hbar} \cdots \frac{dp_{3N}}{2\pi\hbar} \ , \tag{155}$$

and so forth. The element of integration in phase space for degree of freedom i is therefore $dq_i dp_i/h$, where $h = 2\pi\hbar$ is Planck's original constant.

2.3 Canonical Quantization

The first route from classical to quantum mechanics, discovered by Heisenberg, Born, Jordan and Dirac in 1925, is not the only one, but it is the most direct and succinct, and will now be summarized. Its point of departure is classical mechanics in the Hamiltonian format, that is, using canonical coordinates and momenta satisfying first order equations of motion. The leap to quantum mechanics is the replacement of these numbers by Hermitian operators acting on the infinite dimensional Hilbert space $\mathfrak{H}$ of the preceding discussion, and the specification of commutation rules between these operators.

(a) The Canonical Commutation Rules

The system of interest will, to begin with, again be that of N particles in three spatial dimensions treated as if they had no internal structure, i.e., a system with $3N$ degrees of freedom. For each degree of freedom Hermitian coordinate and momentum *operators* q_i and p_i $(i = 1, \ldots, 3N)$ are introduced. Eigenvalues of these operators will be designated by primes: q_i' and p_i'.

These operators are postulated to obey the following *canonical commutation rules*:

$$[q_i, p_j] = i\hbar\, \delta_{ij} \ , \tag{156}$$

$$[q_i, q_j] = 0, \qquad [p_i, p_j] = 0 \ . \tag{157}$$

The q-p commutator is the heart of the matter, and is the point of entry for $\hbar$.

Shortly we will see that symmetry considerations almost suffice to determine the commutation rules, though of course not $\hbar$. For now, we take (156) and (157) for granted and analyze their consequences.

Because all the q's commute, they can be diagonalized simultaneously; the same goes for the p's. On the other hand, q_i and p_j cannot be diagonalized simultaneously if $i = j$. Two sets of simultaneous eigenkets are thus

$$\begin{aligned} |q_1' \ldots q_{3N}'\rangle &\equiv |q_1'\rangle \otimes |q_2'\rangle \ldots \otimes |q_{3N}'\rangle \ , \\ |p_1' \ldots p_{3N}'\rangle &\equiv |p_1'\rangle \otimes |p_2'\rangle \ldots \otimes |p_{3N}'\rangle \ . \end{aligned} \tag{158}$$

In view of this factorization, it suffices to examine just one degree of freedom, with coordinate and momentum operators q and p satisfying

$$[q, p] = i\hbar \ . \tag{159}$$

Repeated use of the commutation rule (159) shows that

$$[q, p^n] = in\hbar p^{n-1}, \qquad [p, q^n] = -in\hbar q^{n-1} \ ; \tag{160}$$

apart from a factor, these right-hand sides have the form of derivatives of p^n and q^n. Motivated by this observation, consider any function $G(p)$ of the operator p that has a power series expansion, such as an exponential of p, and $F(q)$ any function of the operator q of the same type. Eq. 160 then generalizes to the important commutation rules

$$[q, G(p)] = i\hbar \frac{\partial G(p)}{\partial p} \, , \qquad [p, F(q)] = \frac{\hbar}{i} \frac{\partial F(q)}{\partial q} \ . \tag{161}$$

For functions of all the coordinates or momenta, these rules clearly are

$$[q_i, G(p_1 \dots p_{3N})] = i\hbar \frac{\partial G}{\partial p_i} , \qquad [p_i, F(q_1 \dots q_{3N})] = \frac{\hbar}{i} \frac{\partial F}{\partial q_i} . \tag{162}$$

The commutation rules Eq. 161, which are direct consequences of the canonical commutators, lead to an expected conclusion, which is nonetheless important: the spectra of q and p are both continuous from $-\infty$ to ∞. To demonstrate this, introduce the unitary operator

$$T(a) = e^{-iap/\hbar} , \tag{163}$$

where a is any real number having the dimension of length. $T(a)$ is unitary because p is Hermitian. Then, because of (161),

$$qT(a) = T(a)q + i\hbar \partial T/\partial p = T(a)(q + a) . \tag{164}$$

Let $|q'\rangle$ be some eigenket of q

$$q|q'\rangle = q'|q'\rangle , \tag{165}$$

and consider $qT(a)|q'\rangle$, which is

$$qT(a)|q'\rangle = (q' + a)T(a)|q'\rangle , \tag{166}$$

due to (164). Hence $T(a)|q'\rangle$ is an eigenket of q with eigenvalue $q' + a$. But a was arbitrary, and therefore all real numbers are eigenvalues of q.

This argument shows that the unitary operator $T(a)$ produces a *spatial translation* through the distance a. That is, by multiplying (164) by $T^\dagger$,

$$T^\dagger(a) q T(a) = q + a , \tag{167}$$

which is the unitary transformation of the coordinate operator corresponding to a spatial translation. Because T is unitary, it preserves norms, and therefore (166) implies

$$T(a)|q'\rangle = |q' + a\rangle . \tag{168}$$

This recognition that $T(a)$ produces a translation of the coordinate operators q_i and their eigenkets implies that *symmetry considerations largely determine the canonical commutation rules:* first, the fact that translations along different directions commute requires $[p_i, p_j] = 0$; and second, requiring the coordinates to obey (167) requires $[q_i, p_j] = i\delta_{ij}C$. The last commutation rule, $[q_i, q_j] = 0$, is based on the separate assumption that all coordinate components can be simultaneously specified. While C has the dimension of action, experiment is needed to confirm that C agrees with, for example, the value of $\hbar$ found from fitting the cosmic background radiation with the Planck distribution.

The same argument can be applied to p by use of the unitary operator

$$K(k) = e^{iqk/\hbar} , \tag{169}$$

where k is now any real number having the dimension of momentum. The result is that if $|p'\rangle$ is an eigenket of p with the indicated eigenvalue, so is $|p' + k\rangle$ for all k. The unitary operator $K(k)$ produces a translation in momentum space by k:

$$K^\dagger(k) p K(k) = p + k , \qquad K(k)|p'\rangle = |p' + k\rangle . \tag{170}$$

Translations in momentum space are often referred to as boosts.

Because of their continuous spectra, the coordinate and momentum eigenkets are normalized to delta functions:

$$\langle q'|q''\rangle = \delta(q'-q'')\,, \qquad \langle p'|p''\rangle = \delta(p'-p'')\ . \tag{171}$$

An important observation regarding the role of time, due to Pauli, is a consequence of the continuous spectra for coordinates and momenta. Were the goal to extend what has been said thus far to a relativistic theory, a first attempt might be to put time on the same footing as the spatial coordinates by generalizing the commutation rule to one between 4-vectors for position and momentum. This would imply the time-energy commutator

$$[\hat{t}, H] = -i\hbar\ , \tag{172}$$

where $\hat{t}$ is a Hermitian operator whose eigenvalues are time, H is the energy operator (the Hamiltonian), and the sign is chosen on the supposition that the coordinates and momenta are 4-vectors. But as we just saw, if $\hat{t}$ is to have a continuous spectrum like the coordinates, then so must H; i.e., there could be no lower bound to energies and no bound states with discrete energies! So this path to a relativistic theory is a disaster at the start. Indeed, what is done in relativistic quantum mechanics is to demote the spatial coordinates from operators to the same status as time, as 4-vector *parameters* that label observables such as the electromagnetic field operators to be discussed in chapter 10. That the coordinates are not eigenvalues of operators in relativistic quantum mechanics is consistent with the fact, pointed out in §1.1, that the position of a particle of mass m cannot be determined to an accuracy better than the Compton wave length $\hbar/mc$.

(b) Schrödinger Wave Functions

Schrödinger's originally distinct formulation of quantum mechanics in terms of wave functions and differential operators follows from canonical quantization by writing all operator and kets in the coordinate representation. In particular, the Schrödinger wave function is the scalar product $\langle q_1' \ldots |\psi\rangle$.

The key is the transformation function between the coordinate and momentum representations for one degree of freedom, $\langle q'|p'\rangle$, that is to say, the wave function when $|\psi\rangle$ is actually $|p'\rangle$. Let $|0_q\rangle$ and $|0_p\rangle$ be the eigenkets of q and p with eigenvalue 0. Then by use of the unitary operators T and K,

$$\begin{aligned}\langle q'|p'\rangle = \langle 0_q|T^\dagger(q')|p'\rangle &= e^{iq'p'/\hbar}\langle 0_q|p'\rangle \\ &= e^{iq'p'/\hbar}\langle 0_q|K(p')|0_p\rangle = e^{iq'p'/\hbar}\langle 0_q|0_p\rangle\ .\end{aligned} \tag{173}$$

The constant $\langle 0_q|0_p\rangle$ is determined, up to an arbitrary phase, by requiring

$$\int dp'\,\langle q'|p'\rangle\langle p'|q''\rangle = \delta(q'-q'')\ , \tag{174}$$

and by recalling the Fourier representation of the delta function:

$$\int \frac{dq'}{2\pi\hbar} e^{ip'q'/\hbar} = \delta(p')\ . \tag{175}$$

The phase is then chosen so as to produce

$$\langle q'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip'q'/\hbar} = \varphi_{p'}(q') \ , \tag{176}$$

to return to the notation of Eq. 74. Hence for the N-particle system the wave function when all particles are in momentum eigenstates is a product of plane waves:

$$\langle q'_1 \ldots | p'_1 \ldots \rangle = (2\pi\hbar)^{-3N/2} \prod_{i=1}^{3N} e^{ip_i q_i/\hbar} \ . \tag{177}$$

Configuration and momentum space wave functions are defined as scalar products of $|\psi\rangle$ with coordinate and momentum eigenkets:

$$\psi(q') = \langle q'|\psi\rangle, \qquad \phi(p') = \langle p'|\psi\rangle \ . \tag{178}$$

Hence

$$\phi(p') = \int dq' \, \langle p'|q'\rangle\langle q'|\psi\rangle \ , \tag{179}$$

which is just the Fourier transform of $\psi(q')$ because of (176):

$$\phi(p') = \int \frac{dq'}{\sqrt{2\pi\hbar}} e^{-ip'q'/\hbar} \, \psi(q') \ ; \tag{180}$$

its inverse is

$$\psi(q') = \int \frac{dp'}{\sqrt{2\pi\hbar}} e^{ip'q'/\hbar} \, \phi(p') \ . \tag{181}$$

The probability distributions in configuration and momentum space are then $|\psi(q')|^2$ and $|\phi(p')|^2$. Given one it is *not* possible to construct the other. This is so because the probabilities only depend on the modulus of the wave functions, and phases that depend on either q' or p' must be known for the transformation from one representation to the other. The density matrix in any one representation does, of course, suffice, to determine that in any the other. In this context,

$$\langle q'|\rho|q''\rangle = \psi(q')\psi^*(q'') \, , \qquad \langle p'|\rho|p''\rangle = \phi(p')\phi^*(p'') \ , \tag{182}$$

and therefore

$$\langle p'|\rho|p''\rangle = \int \frac{dq'dq''}{2\pi\hbar} \, e^{-i(p'q'-p''q'')/\hbar} \, \langle q'|\rho|q''\rangle \ . \tag{183}$$

In short, to compute the momentum distribution $\langle p'|\rho|p'\rangle$ one must know the off-diagonal elements of ρ in the coordinate representation.

This example illustrates a general property of quantum mechanical probability distributions: *the probability distribution for a complete set of compatible observables does not determine the probability distribution for an incompatible observable.*

To determine the action of the momentum operator on configuration space wave functions the matrix elements of p in the q-representation is needed:

$$\langle q'|p^n|q''\rangle = \int dp' \, \langle q'|p'\rangle (p')^n \langle p'|q''\rangle = \int \frac{dq'}{2\pi\hbar} (p')^n \, e^{ip'(q'-q'')/\hbar} \ . \tag{184}$$

This is the nth derivative of a delta function:

$$\delta^{(n)}(x) = \frac{d^n}{dx^n}\delta(x) = \int dk\,(ik)^n\,e^{ikx}\ , \tag{185}$$

which has the property

$$\frac{d^n f(x)}{dx^n} = \int dx'\,\delta^{(n)}(x-x')f(x') \tag{186}$$

for a function that is sufficiently continuous at x. Hence (184) is

$$\langle q'|p^n|q''\rangle = (\hbar/i)^n\,\delta^{(n)}(q'-q'')\ , \tag{187}$$

and therefore

$$\langle q'|p^n|\psi\rangle = \left(\frac{\hbar}{i}\frac{\partial}{\partial q'}\right)^n\,\psi(q')\ . \tag{188}$$

The same argument gives the corresponding result for the action of coordinate operators on wave functions in momentum space:

$$\langle p'|q^n|\psi\rangle = \left(i\hbar\frac{\partial}{\partial p'}\right)^n\,\phi(p')\ . \tag{189}$$

The generalization of these formulas to more than one degree of freedom is straightforward and will not be spelled out. There is, however, one aspect of the extension to many degrees of freedom that merits attention: the displacement of *all* the coordinates. To construct the unitary operator that does this, we must group the three coordinates and momenta of each particle into vector operators: $\boldsymbol{x}_1 = (q_1, q_2, q_3)$, $\boldsymbol{x}_2 = (q_4, q_5, q_6)$, etc., and similarly with the momenta, which we now enumerate as $\boldsymbol{x}_n$, $\boldsymbol{p}_n$, with $n = 1, \ldots, N$. The displacement by the 3-vector $\boldsymbol{a}$ is to be produced by a unitary operator $T(\boldsymbol{a})$ that generalizes $T(a)$, as given by (163), so that (167) is replaced by

$$T^\dagger(\boldsymbol{a})\boldsymbol{x}_n T(\boldsymbol{a}) = \boldsymbol{x}_n + \boldsymbol{a}\ , \tag{190}$$

with $\boldsymbol{a}$ the same for all n. Because all individual momentum components commute with each other, T is simply a product of the operators T for each degree of freedom with the component of $\boldsymbol{a}$ appropriate to the momentum component in question, i.e.,

$$T(\boldsymbol{a}) = \prod_{n=1}^{N} \exp(-i\boldsymbol{p}_n\cdot\boldsymbol{a}/\hbar)\ . \tag{191}$$

But

$$\boldsymbol{P} = \sum_{n=1}^{N}\boldsymbol{p}_n \tag{192}$$

is the total momentum. Thus the spatial displacement operator for the whole system can written in terms of the total momentum as

$$T(\boldsymbol{a}) = e^{-i\boldsymbol{P}\cdot\boldsymbol{a}/\hbar}\ . \tag{193}$$

(c) Uncertainty Relations

The Heisenberg uncertainty relation for coordinates and momenta is but one example of such relations that hold for all pairs of incompatible observables.

To derive such relations, a precise definition of the uncertainty ΔA of an observable A is needed. The convenient and physically reasonable choice is the root-mean-square (rms) dispersion ΔA, defined as

$$\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2} \ , \tag{194}$$

where $\langle \ldots \rangle$ is the expectation value in an arbitrary ket $|\phi\rangle$, i.e.,

$$(\Delta A)^2 = \sum_a (a - \langle A \rangle)^2 \, |\langle a|\phi \rangle|^2 \ , \tag{195}$$

which is the second moment of the probability distribution $|\langle a|\phi\rangle|^2$.

Let B be an observable that does not commute with A. The goal is to find a lower bound for $\Delta A \, \Delta B$ as the precise statement of the uncertainty principle for arbitrary observables. For that purpose it proves to be convenient to define

$$\bar{A} = A - \langle A \rangle, \qquad \bar{B} = B - \langle B \rangle \ , \tag{196}$$

$$\bar{A}|\phi\rangle = |\phi_A\rangle, \qquad \bar{B}|\phi\rangle = |\phi_B\rangle \ . \tag{197}$$

Then

$$(\Delta A \, \Delta B)^2 = \langle \phi_A | \phi_A \rangle \langle \phi_B | \phi_B \rangle \ , \tag{198}$$

which, due to the Schwarz inequality (Eq. 17) gives

$$(\Delta A \, \Delta B)^2 \geq |\langle \bar{A} \bar{B} \rangle|^2 \ . \tag{199}$$

Now

$$\bar{A}\bar{B} = \tfrac{1}{2}[A, B] + \tfrac{1}{2}\{\bar{A}, \bar{B}\} = \tfrac{1}{2} i C + \tfrac{1}{2}\{\bar{A}, \bar{B}\} \ , \tag{200}$$

where C and the anticommutator are both Hermitian. Hence

$$(\Delta A \, \Delta B\rangle)^2 \geq \tfrac{1}{4} |\langle \{\bar{A}, \bar{B}\} \rangle + i \langle C \rangle|^2 \ , \tag{201}$$

and as both expectation values are real,

$$(\Delta A \, \Delta B\rangle)^2 \geq \tfrac{1}{4} \langle \{\bar{A}, \bar{B}\} \rangle^2 + \tfrac{1}{4} \langle C \rangle^2 \ , \tag{202}$$

As shown by Prob. 6, when $|\phi\rangle$ is chosen to make $|\phi_A\rangle$ proportional to $|\phi_B\rangle$, the first term in (202) vanishes; therefore

$$\Delta A \, \Delta B \geq \tfrac{1}{2} |\langle [A, B] \rangle| \ . \tag{203}$$

This is *the general form of Heisenberg's uncertainty relation.* For the canonical variables, it reads

$$\Delta p_i \, \Delta q_j \geq \tfrac{1}{2} \hbar \, \delta_{ij} \ , \tag{204}$$

which now gives a precise lower bound in place of the order-of-magnitude estimate of §1.1.

Because time cannot be the eigenvalue of an operator, it is now clear that the time-energy uncertainty relation has a quite different meaning from that for quantities represented by operators. It will, therefore, be discussed separately in §2.4.

2.4 The Equations of Motion

What might be called kinematics is all that has been considered thus far. How states evolve in time will now be addressed.

(a) The Schrödinger Picture

The basic assumption will be that time evolution is represented by a unitary transformation parametrized by a continuous parameter t . If the superposition principle is taken to be fundamental, this assumption is almost inescapable, because superposition requires time evolution to be a linear transformation of vectors in the Hilbert space, i.e., if $|\psi;0\rangle$ is some state of a system at $t=0$, then at a later time $|\psi;t\rangle = L_t|\psi;0\rangle$, where L_t is a linear operator.

Consider some *time-independent* observable, A, with the spectrum $(a, a', \ldots)$. Its expectation value as a function of time will be

$$\langle\psi;t|A|\psi;t\rangle = \sum_a a|\langle\psi;t|a\rangle|^2 \ . \tag{205}$$

In general, the probabilities $|\langle\psi;t|a\rangle|^2$ for the various eigenvalues will change with time, but by hypothesis, not the eigenvalues themselves. On the other hand, rewriting (205) in terms of the operator L_t gives

$$\langle\psi;0|L_t^\dagger A L_t|\psi;0\rangle = \sum_{a_t} a_t|\langle\psi;0|a_t\rangle|^2 \ , \tag{206}$$

where $\{|a_t\rangle\}$ are the eigenkets of $L_t^\dagger A L_t$ and $\{a_t\}$ its eigenvalues. As just said, however, the spectrum must not change with time, whereas the probabilities can. But any unitary transformation of a Hermitian operator leave its spectrum invariant, and it is this fact that justifies the assumption that L_t is a unitary operator. Accepting this assumption means that there is a unitary operator $U(t',t)$ that manufactures $|\psi;t'\rangle$ from the state at time t:

$$|\psi;t'\rangle = U(t',t)|\psi;t\rangle \ . \tag{207}$$

Consider first a system that is isolated from external disturbances, so that the origin of time has no physical significance. When this is so, U simplifies greatly because it can only depend on time differences:

$$|\psi;t'\rangle = U(t'-t)|\psi;t\rangle \ . \tag{208}$$

These unitary operators must satisfy the following composition law:

$$U(t_2)U(t_1) = U(t_2+t_1) \ . \tag{209}$$

The crucial point here is that the composite is a function of the sum t_1+t_2, and therefore

$$U(t) = [U(t/N)]^N \ . \tag{210}$$

Now as $\delta t \to 0$, $U(\delta t) \to 1$, and therefore $U(\delta t) = 1 - i\Delta(\delta t)$, where $\Delta(\delta t)$ must be an infinitesimal Hermitian operator so as to make U unitary to first order in Δ.

The composition law (209) implies that $\Delta(\delta t_1) + \Delta(\delta t_2) = \Delta(\delta t_1 + \delta t_2)$, i.e., that $\Delta(\delta t)$ is proportional to δt. This fact is expressed by

$$U(\delta t) = 1 - i\delta t H/\hbar \ , \tag{211}$$

where $\hbar$ is introduced so that the operator H has the dimension of energy. It is *the Hamiltonian* of the system in question.

For finite time differences, (210) gives

$$U(t) = [U(t/N)]^N = \lim_{N\to\infty} \left(1 - \frac{1}{N}\frac{itH}{\hbar}\right)^N \ , \tag{212}$$

and therefore

$$U(t) = e^{-iHt/\hbar} \ . \tag{213}$$

An equivalent derivation is

$$U(t+\delta t) - U(t) = [U(\delta t) - 1]U(t) = -i(\delta t H/\hbar)U(t) \ , \tag{214}$$

so that

$$i\hbar \frac{\partial}{\partial t} U(t) = H\, U(t) \ , \tag{215}$$

which has the solution (213) because of the initial condition $U(0) = 1$. Because of its role in the unitary operator $U(t)$, the Hamiltonian is called the generator of translations in time.

The *Schrödinger equation* then follows from (207) and (215):

$$i\hbar \frac{\partial}{\partial t} |\psi; t\rangle = H|\psi; t\rangle \ . \tag{216}$$

The case of an eigenstate of H is of particular importance, i.e., a ket $|\psi_E; t\rangle$ that satisfies the *time-independent Schrödinger equation*

$$(H - E)|\psi_E; t\rangle = 0 \ . \tag{217}$$

The solution of (216) is then trivial:

$$|\psi_E; t\rangle = e^{-iEt/\hbar}|\psi_E; 0\rangle \ . \tag{218}$$

Energy eigenstates are called *stationary states* because they do not change in time, aside from a phase factor. Furthermore, the matrix elements of any time-independent observable A between stationary states also have a time dependence that is merely a phase:

$$\langle \psi_E; t|A|\psi_{E'}; t\rangle = e^{i(E-E')t/\hbar} \langle \psi_E; 0|A|\psi_{E'}; 0\rangle \ . \tag{219}$$

It is a mathematically trivial, but nonetheless important fact that for any operator A

$$\langle \psi_E|[A, H]|\psi_E\rangle = 0 \ ; \tag{220}$$

in words, that the commutator of any observable with the Hamiltonian has zero expectation value in all stationary states.

Consider an N-particle system with a Hamiltonian that has the form familiar from classical mechanics when the forces are velocity-independent:

$$H = \sum_{n=1}^{N} \frac{\boldsymbol{p}_n^2}{2m_n} + V(\boldsymbol{x}_1 \ldots \boldsymbol{x}_N) \ . \tag{221}$$

Here $\boldsymbol{x}_n$ is the coordinate operator for particle n; its eigenvalues will be designated by $\boldsymbol{r}_n$. To put (216) into the coordinate representation, one takes the scalar product with a coordinate eigenket $|\boldsymbol{r}_1 \ldots \boldsymbol{r}_N\rangle$. For this purpose recall Eq. 188, which in the present notation is

$$\langle \boldsymbol{r}_1 \ldots |\boldsymbol{p}_n|\psi;t\rangle = \frac{\hbar}{i}\frac{\partial}{\partial \boldsymbol{r}_n}\psi(\boldsymbol{r}_1 \ldots ;t) \ . \tag{222}$$

This then gives *the Schrödinger equation in the coordinate representation:*

$$i\hbar\frac{\partial}{\partial t}\psi(t) = \left(\sum_n \frac{1}{2m_n}\left(\frac{\hbar}{i}\frac{\partial}{\partial \boldsymbol{r}_n}\right)^2 + V(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N)\right)\psi(t) \ . \tag{223}$$

If the classical Hamiltonian does not have the simple form (221), and contains expressions like qp, there is no unique recipe for turning it into a Hermitian operator. One obvious possibility is $qp \to \frac{1}{2}(qp + pq)$, but there are others. This ambiguity vanishes as $\hbar \to 0$, and by the same token classical mechanics does not always provide a clearcut rule for the move to quantum mechanics because anything that vanishes as $\hbar \to 0$ is invisible in the classical limit. It is remarkable that in so much of physics the unmodified classical Hamiltonian can be taken over successfully into quantum mechanics.

The unitary nature of time evolution leads to conservation laws and continuity equations involving the probability. These all stem from the following immediate consequence of Eq. 207: *the scalar product of any two solutions of the time-dependent Schrödinger equation is independent of time.*

The constancy in time of the norm $\langle\psi;t|\psi;t\rangle$ is perhaps the most important example. In terms of the coordinate space probability distribution,

$$w(\boldsymbol{r}_1, \ldots ;t) \equiv |\psi(\boldsymbol{r}_1, \ldots ;t)|^2 \ , \tag{224}$$

the constancy of the norm is

$$\frac{\partial}{\partial t}\int d^3r_1 \ldots d^3r_N \ w(\boldsymbol{r}_1, \ldots ;t) = 0 \ . \tag{225}$$

If the interactions are diagonal in the coordinate representation, a much stronger statement holds in any infinitesimal region of configuration space, namely,

$$\frac{\partial}{\partial t}\, w(\boldsymbol{r}_1 \ldots ;t) + \sum_{n=1}^{N} \frac{\partial}{\partial \boldsymbol{r}_n} \cdot \boldsymbol{i}_n(\boldsymbol{r}_1 \ldots ;t) = 0 \ , \tag{226}$$

where

$$\boldsymbol{i}_n(\boldsymbol{r}_1 \ldots) = \frac{\hbar}{2im_n}\left(\psi^*\frac{\partial\psi}{\partial \boldsymbol{r}_n} - \psi\frac{\partial\psi^*}{\partial \boldsymbol{r}_n}\right) \ . \tag{227}$$

This is a continuity equation in the $3N$-dimensional configuration space, *not* in everyday 3-space, $\mathfrak{E}_3$; the N-tuple of 3-vectors $\boldsymbol{i}_n$ is needed to describe flow across a hypersurface in configuration space, and reflects the fact that the Schrödinger equation is a wave equation in configuration space, and only a conventional wave equation in the case of one particle. The global conservation law (Eq. 225) follows from the local law (226), if the wave function falls off sufficiently at large distances to have a finite norm.

In the important case of a stationary state, i.e., when $\partial w/\partial t = 0$, the continuity equation reduces to the condition that the current is divergence free:

$$\sum_n \frac{\partial}{\partial \boldsymbol{r}_n} \cdot \boldsymbol{i}_n = 0 \; . \tag{228}$$

To derive (226), note that (216) implies

$$-i\hbar\partial_t \langle \psi; t| = \langle \psi; t|H \tag{229}$$

because H must be Hermitian if probability is to be conserved. Using the shorthand $i\hbar\partial_t \langle \boldsymbol{r}|\psi\rangle = \langle \boldsymbol{r}|H|\psi\rangle$, etc.,

$$i\hbar\partial_t |\psi(\boldsymbol{r})|^2 = \langle\psi|\boldsymbol{r}\rangle\langle\boldsymbol{r}|H|\psi\rangle - \langle\psi|H|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\psi\rangle \; . \tag{230}$$

The potential energy V does not contribute to the right-hand side because it is assumed to be diagonal in the coordinate representation; the kinetic energy K gives:

$$\psi^*(\boldsymbol{r})\langle\boldsymbol{r}|K|\psi\rangle - \langle\psi|K|\boldsymbol{r}\rangle\psi(\boldsymbol{r}) = -\sum_n \frac{\hbar^2}{2m_n} \frac{\partial}{\partial \boldsymbol{r}_n} \cdot \left(\psi^* \frac{\partial}{\partial \boldsymbol{r}_n}\psi - \psi \frac{\partial}{\partial \boldsymbol{r}_n}\psi^* \right), \tag{231}$$

which establishes (226).

If the particles in question are electrically charged, expressions for conventional charge and current densities, ρ and $\boldsymbol{j}$, are often needed. These are

$$\rho(\boldsymbol{r}, t) = \sum_n e_n \int d^3r_1 \ldots d^3r_N \; \delta(\boldsymbol{r} - \boldsymbol{r}_n) \, |\psi(\boldsymbol{r}_1 \ldots; t)|^2 \, , \tag{232}$$

$$\boldsymbol{j}(\boldsymbol{r}, t) = \sum_n e_n \int d^3r_1 \ldots d^3r_N \; \delta(\boldsymbol{r} - \boldsymbol{r}_n) \; \boldsymbol{i}_n(\boldsymbol{r}_1 \ldots; t) \; . \tag{233}$$

The proof that this density and current satisfy the conventional continuity equation in $\mathfrak{E}_3$ is left as an exercise.

The constancy of the scalar product $\langle \psi_1; t|\psi_2; t\rangle$ for two solutions of one Schrödinger equation is also accompanied by a continuity equation when the interaction is local:

$$\frac{\partial}{\partial t}\psi_1^*\psi_2 + \sum_n \frac{\hbar}{2im_n} \frac{\partial}{\partial \boldsymbol{r}_n} \cdot \left(\psi_1^* \frac{\partial \psi_2}{\partial \boldsymbol{r}_n} - \psi_2 \frac{\partial \psi_1^*}{\partial \boldsymbol{r}_n} \right) = 0 \; . \tag{234}$$

The proof is again left as an exercise.

Thus far we have dealt with the time development of pure states. Let $\{|a\rangle\}$ be a basis that diagonalizes the density matrix at $t = 0$:

$$\rho(0) = \sum_a |a\rangle p_a \langle a| \; . \tag{235}$$

At later times, $|a\rangle \to \exp(-iHt/\hbar)|a\rangle$, and therefore,

$$\rho(t) = e^{-iHt/\hbar}\rho(0)\, e^{iHt/\hbar} \ . \tag{236}$$

Note that the probabilities p_a do not change with time. The equation of motion for the density matrix follows by differentiating (236):

$$i\hbar\frac{d}{dt}\rho(t) = [H, \rho(t)] \ . \tag{237}$$

This is an important equation, especially in statistical physics. Loosely speaking, it is the counterpart of Liouville's equation in classical mechanics, though of course the latter pertains to phase space.

Finally, consider a system exposed to time-dependent applied forces. The origin of time is then no longer arbitrary, and the unitary time evolution operator $U(t', t)$ depends on both of its arguments, not just the interval $t' - t$. These operators now have the composition law

$$U(t'', t')U(t', t) = U(t'', t) \ , \tag{238}$$

which states that evolving to t' followed by evolving to t'' is the same as evolving directly from t to t''. The first question is whether infinitesimal transformations can still be written in the form of Eq. 211. To answer this, specialize (238) to two infinitesimal time increments:

$$U(t + \delta_2 + \delta_1, t + \delta_1)U(t + \delta_1, t) = U(t + \delta_2 + \delta_1, t) \ . \tag{239}$$

But $U(t + \delta, t) = 1 - iF(t, \delta)$ for an infinitesimal δ, with F being an infinitesimal Hermitian operator, and so (239) requires $F(t, \delta_2) + F(t, \delta_1) = F(t, \delta_2 + \delta_1)$, i.e., that $F(t, \delta)$ be proportional to δ. Hence in this case

$$U(t + \delta t, t) = 1 - i\delta t\, H(t)/\hbar \ , \tag{240}$$

where $H(t)$ is the *time-dependent Hamiltonian.* Therefore

$$U(t + \delta t, t') = U(t, t') - i\delta t H(t)U(t, t')/\hbar \ , \tag{241}$$

and so the differential equation (215) holds in the following form

$$i\hbar\frac{\partial}{\partial t}U(t, t') = H(t)U(t, t') \ . \tag{242}$$

Hence the Schrödinger equation for a time-dependent Hamiltonian still has the form of Eq. 216, and the scalar product of any two of its solutions is time-independent.

While the differential equation for $U(t, t')$ seems to be identical to the one for a time-independent Hamiltonian, that would be a misperception: in general, it is no longer possible to integrate the equation even in the formal manner that previously led to $\exp(-iHt/\hbar)$ to obtain $U(t, t')$ for finite time differences because, in most situations of physical interest, $H(t)$ does not commute with $H(t')$ when $t \neq t'$. (Recall that what made the integration possible (indeed, trivial) in the time-independent case was that H then behaved like a number.) A major industry has been devoted for decades to grappling with this time-dependent situation, because even when the system is isolated and the complete Hamiltonian is time-independent the perverse notion of turning the problem into a time-dependent one proves to be very fruitful, as we will see in subsection (e).

(b) The Heisenberg Picture

In the preceding discussion of time dependence, the state vector or density matrix changed with time, while the observables did not (unless, of course, they are explicitly time-dependent like the Hamiltonian $H(t)$ in Eq. 242.) Because time evolution is unitary, another equivalent formulation, in which the observables move while the state stays put, is also available. The former, where the states move is called the *the Schrödinger picture,* and the latter where they do not but the observables move, *the Heisenberg picture.* The Heisenberg picture is better suited to bringing out fundamental features, such as symmetries and conservation laws, and it is indispensable in systems with many degrees of freedom, like those dealt with in quantum field theory and statistical physics.

Assume a time-independent Hamiltonian, so that $U(t) = \exp(-iHt/\hbar)$. The case where H depends on t is not different in principle, but of course more complicated. Let $\{|\psi_b; t\rangle\}$ be a complete set of solutions of the Schrödinger equation, and call their $t = 0$ values $|\psi_b\rangle$. The matrix elements of a time-independent observable A in this moving basis are

$$\langle\psi_b; t|A|\psi_{b'}; t\rangle = \langle\psi_b|e^{iHt/\hbar}Ae^{-iHt/\hbar}|\psi_{b'}\rangle \ . \tag{243}$$

This tells us how to put the burden of carrying the time-dependence on the observables:

- *In the Heisenberg picture, kets that describe the time evolution of pure states are fixed in the Hilbert space, and observables A that are time-independent in the Schrödinger picture are replaced by operators $A(t)$ that evolve with the unitary transformation*

$$A(t) = e^{iHt/\hbar}\, A\, e^{-iHt/\hbar} \ . \tag{244}$$

Observables in the Heisenberg picture therefore obey the equation of motion

$$i\hbar\frac{d}{dt}\, A(t) = [A(t), H] \ . \tag{245}$$

This equation has two immediate consequences of great importance:

- *Observables that commute with the Hamiltonian are constants of motion.*
- *Any one constant of motion can be diagonalized simultaneously with the Hamiltonian, i.e, they possess simultaneous eigenstates. The Hamiltonian and a set of constants of motion can be diagonalized simultaneously provided that all these constants of motion commute with each other.*

One should not be misled by the superficial similarity between the equation of motion for ρ in the Schrödinger picture (Eq. 237) and the Heisenberg picture equation (245). *The density matrix does not move in the Heisenberg picture,* because the kets that describe the pure states that define ρ (e.g., as in Eq. 235) are fixed in this picture.

When the Hamiltonian has the familiar form of Eq. 221, the commutation rules (162) immediately yield the following equations of motion for the canonical coordinates and momenta in the Heisenberg picture:

$$\frac{dq_i(t)}{dt} = \frac{\partial H}{\partial p_i} \ , \qquad \frac{dp_i(t)}{dt} = -\frac{\partial H}{\partial q_i} \ . \tag{246}$$

These have exactly the same form as Hamilton's classical equations of motion.

Of course, integration of the quantum mechanical equations is, in general, a far more difficult proposition because the dynamical variables do not commute with each other. This complication is partially absent, however, if the Hamiltonian has the conventional form (221) and V has only linear and quadratic terms in the coordinates, for then the equations of motion are linear:

$$\dot{q}_i = p_i/m_i, \qquad \dot{p}_i = a_i + \sum_j \omega_{ij} q_j \ . \tag{247}$$

Hence the expectation values of q_i and p_i in any state, whether pure or mixed, evolve exactly like those of classical mechanics for the important cases of no forces, a constant force, and harmonic motion. Of course, this does not mean that there is then no difference between classical and quantum mechanics.

It should be noted that a ket $|\alpha\rangle_S$ that is stationary in the Schrödinger picture will become the moving ket $|\alpha(t)\rangle_H = U^\dagger(t)|\alpha\rangle_S$ in the Heisenberg picture. Furthermore, if an observable $B_S(t)$ is explicitly time-dependent in the Schrödinger picture, its counterpart in the Heisenberg picture is still given by (244) but obeys the equation of motion

$$i\hbar \frac{d}{dt} B_H(t) = i\hbar \frac{\partial}{\partial t} B_H(t) + [B_H(t), H] \ . \tag{248}$$

Finally, should the Hamiltonian $H_S(t)$ itself be time-dependent in the Schrödinger picture, the transformation (244) is replaced by

$$A_H(t,t') = U^\dagger(t,t') A_S U(t,t') \ , \tag{249}$$

and this also applies to the Hamiltonian. Consequently the equation of motion (245) becomes

$$i\hbar \frac{d}{dt} A_H(t,t') = [A_H(t,t'), H_H(t,t')] \ . \tag{250}$$

This situation is illustrated by the interaction picture, which is to be treated in §2.4(e).

(c) Time Development of Expectation Values

The Heisenberg picture is well suited to addressing the question of how expectation values evolve in time quite generally. For the Hamiltonian (221), the Heisenberg equations of motion are

$$\frac{dq_i(t)}{dt} = \frac{1}{m_i} p_i(t) \ , \qquad \frac{dp_i(t)}{dt} = -\frac{\partial V}{\partial q_i} \equiv F_i \ , \tag{251}$$

where F_i is the force operator.

Let $\bar{q}_i(t)$, etc., denote the expectation values $\langle q_i(t)\rangle$ in an arbitrary state. Then

$$\frac{d\bar{p}_i(t)}{dt} = \langle F(q_1(t) \ldots, q_f(t))\rangle \ , \qquad \frac{d\bar{q}_i(t)}{dt} = \frac{1}{m_i} \bar{p}_i(t) \ . \tag{252}$$

These would be Newton's equations for the expectation values if the following replacement were valid:

$$\langle F\rangle \longrightarrow F(\bar{q}_1, \ldots, \bar{q}_f) \ , \tag{253}$$

where it is to be understood that the $\bar{q}_i$ are time-dependent. To see what this approximation would entail, expand the force operator about the expectation values of the coordinates:

$$F_i(q) = F_i(\bar{q}) + \sum_j (q_j - \bar{q}_j)\left.\frac{\partial F_i}{\partial q_j}\right|_{\bar{q}} + \frac{1}{2}\sum_{jk}(q_j - \bar{q}_j)(q_k - \bar{q}_k)\left.\frac{\partial^2 F_i}{\partial q_j \partial q_k}\right|_{\bar{q}} + \dots \ . \quad (254)$$

The linear term in the deviation from $\bar{q}_i$ drop out when the expectation value is taken, which then results in approximate equations for the expectation values of the momenta:

$$\frac{d\bar{p}_i}{dt} \simeq F_i(\bar{q}) + \frac{1}{2}\sum_{jk}\Delta_{jk}(t)\left.\frac{\partial^2 F_i}{\partial q_j \partial q_k}\right|_{\bar{q}} \ , \quad (255)$$

where

$$\Delta_{ij}(t) = \langle q_i(t) q_j(t)\rangle - \bar{q}_i(t)\bar{q}_j(t) \ . \quad (256)$$

Once again, we see that *there are no corrections unless the forces are nonlinear.*

The size of the correction term in (256) depends both on the state and the forces. No generally valid statement about its magnitude can be made. This can already be seen in the simplest case, that of a free particle. In this case (see Prob. 8)

$$\langle q_i^2(t)\rangle - \langle q_i^2(0)\rangle = \frac{t}{m_i}\langle q_i(0)p_i + p_i q_i(0)\rangle + \frac{t^2}{m_i^2}\langle p_i^2\rangle \ , \quad (257)$$

where there is *no sum* over the index i, and the coordinate system is chosen so as to make $\bar{p}_i = \bar{q}_i(0) = 0$. Hence for large values of t,

$$\Delta q_i(t) \longrightarrow t\,\frac{\Delta p_i}{m_i} \gtrsim t\,\frac{\hbar}{m_i \Delta q_i(0)} \ , \quad (258)$$

where the latter is based on the uncertainty principle. The rate at which the quantum mechanical spreading grows is therefore inversely proportional to both the mass and the initial spread. It should be noted, however, that in this force-free case, the spreading is just that of a set of classical free particle trajectories with initial spreads $\Delta q_i(0)$, $\Delta p_i(0)$. In this case, the appearance of $\hbar$ in (258) is due entirely to the requirement that the initial spreads satisfy the uncertainty principle.

(d) Time-Energy Uncertainty

Because it is not possible to define a sensible operator that has time as its spectrum, the time-energy uncertainty relationship is not expressible as one unambiguous theorem to which all must agree, as is the case for uncertainty relationships between the canonical variables and other pairs of dynamical observables.

Nevertheless, given a dynamical system it is usually possible to define one or more operators that play the role of a clock. A vivid and instructive example is the motion of a particle of charge e and mass m in a uniform magnetic field $\boldsymbol{B}$, a problem that will be solved in detail in §4.3. The classical Hamiltonian for motion in the $x - y$ plane perpendicular to the field is

$$H = \tfrac{1}{2}(\dot{x}^2 + \dot{y}^2) \ . \quad (259)$$

This is a quadratic form, and the detailed quantum mechanical solutions are not needed for our purpose: by the theorem stated following Eq. 247, the mean values of the dynamical variables in any wave packet move classically, i.e., with constant angular velocity ω_c on circles, where $\omega_c = eB/mc$ is the cyclotron frequency. This system will therefore toll time with an accuracy ΔT proportional to the sharpness of the clock hand, which is the angular width $\Delta\theta$ of the packet. The natural definition is $\Delta T = \Delta\theta/\omega_c$, so that ΔT equals the period when $\Delta\theta = 2\pi$.

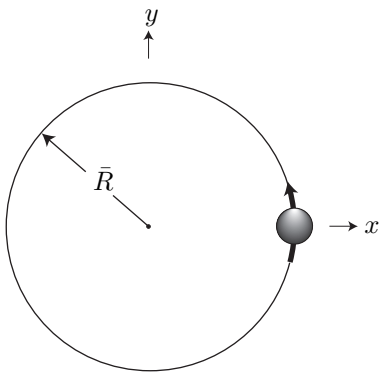

FIG. 2.2. A quantum clock formed by a charged particle wave packet moving in a homogeneous magnetic field perpendicular to the plane of the page.

A definition of $\Delta\theta$ in terms of the dynamical variables is needed which does not suffer from the singularities that afflict trigonometry, such as $\theta = \arctan y/x$. For that reason, we choose a coordinate system whose origin is at the center of the circle, and such that at the instant t of interest the packet is then passing across the x-axis (see Fig. 2.2). Angular positions within a packet are at that instant given by $y/\bar{R}$, where $\bar{R}$ is the r.m.s. radius of the circular orbit. We therefore define a "time" operator T, whose dispersion will be a measure of the clock's precision, by

$$T = y/\bar{R}\omega_c \ . \tag{260}$$

The general uncertainty relation for non-commuting observables (Eq. 203) when applied to such a non-stationary state, then gives

$$\Delta T \, \Delta E \geq \frac{1}{2\bar{R}\omega_c} \, |\langle [y, H] \rangle| \geq \frac{\hbar}{2\bar{R}\omega_c} \, \langle \dot{y} \rangle \tag{261}$$

because of (245). Continuing to take advantage of the classical solution, we have $\langle \dot{y} \rangle \simeq \bar{R}\omega_c$, where we have refrained from an equal sign because we are glossing over any difference between the mean and the r.m.s. radius. With this caveat, we have

$$\Delta T \, \Delta E \gtrsim \tfrac{1}{2} \, \hbar \ . \tag{262}$$

This is the time-energy uncertainty relation for this particular system with this reasonable, but neither unique nor perfectly precise, definition of the time uncertainty.

An arbitrary wave packet will change in angular size, and so the right-hand side of (261) is, in general, a function of time, a fact that is not reflected in the rough

inequality (262). As we shall learn in §4.3(c), in the case of motion in a uniform magnetic field, there is a special set of packets, called coherent states, which do not change in shape, for which the uncertainty product is therefore constant, and which, furthermore, have the minimal time-energy uncertainty product $\sim \hbar$. This too is a special property of quadratic Hamiltonians.

To generalize from this example, consider an observable $Y(t)$ built from the dynamical variables of the system, which is to serve as the pointer of a dynamical "clock." Then, as in (261),

$$\Delta Y(t)\,\Delta E \geq \tfrac{1}{2}\,|\langle [Y(t),H]\rangle| \geq \tfrac{1}{2}\hbar\,\langle \dot{Y}(t)\rangle\ . \tag{263}$$

Now define

$$\Delta T(t) \equiv \frac{\Delta Y(t)}{\langle \dot{Y}(t)\rangle}\ . \tag{264}$$

Then

$$\Delta T(t)\,\Delta E \geq \tfrac{1}{2}\,\hbar\ . \tag{265}$$

This is a quite general time-energy uncertainty relationship; the quantity $\Delta T(t)$ is a time characteristic both of the system and the state in question, and ΔE is the spread in energy of the stationary states that are superposed to form the state. We have emphasized that, in general, both the numerator and denominator in Eq. 264 are functions of t, so ΔT is only a constant under special conditions. On the other hand, ΔE is time-independent if H is.

Instead of using some observable of the system to act as a clock, the issue can also be phrased as follows. We start at $t = 0$ with a system in a *non-stationary* state $|\Phi\rangle$, and ask for the probability that the evolving system is still in $|\Phi\rangle$ at a later time t:

$$P(t) = |\langle\Phi|e^{-iHt/\hbar}|\Phi\rangle|^2 = \left|\int_0^\infty dE\ e^{-iEt/\hbar}\ w_\Phi(E)\right|^2\ , \tag{266}$$

where

$$w_\Phi(E) = \sum_a |\langle Ea|\Phi\rangle|^2\ , \tag{267}$$

a being the eigenvalues of the observables other than H. There are various ways in which one can characterize the time dependence of $P(t)$, and for general energy distributions w_Φ the analysis involved is a subtle matter.[1] In analogy with (264), we can define the function

$$\tau(t) = \frac{P(t)}{dP(t)/dt}\ . \tag{268}$$

It can then be shown that

$$\langle\tau\rangle\,\Delta E \gtrsim \gamma\,\hbar\ , \tag{269}$$

where $\langle\tau\rangle$ is some useful time average of (268), $(\Delta E)^2 = \langle (H - \langle H\rangle)^2\rangle$, and γ is a number of order 1 that depends somewhat on w_Φ.

Clearly, there is only one circumstance under which the definition (268) gives a function $\tau(t)$ that is time-independent: $P(t) = e^{-t/\tau}$, *the exponential decay law*, with τ called the *lifetime* (not the half life $\tau_{1/2} = \tau \ln 2$). This form of $P(t)$ applies

[1] P. Pfeifer and J. Fröhlich, *Rev. Mod. Phys.* **67**, 759 (1995).

to very high accuracy in many phenomena, and we shall study some examples later in this volume. The spectral density $w_\Phi(E)$ that leads from (266) to the exponential decay law is

$$w_\Phi(E) = \frac{1}{\pi} \frac{\frac{1}{2}\Gamma}{(E-E_0)^2 + \frac{1}{4}\Gamma^2} \ . \tag{270}$$

When $\Gamma \ll E_0$, the integral in (266) is readily evaluated (Prob. 7), and gives

$$P(t) = e^{-\Gamma t/\hbar} \ , \tag{271}$$

or

$$\tau = \hbar/\Gamma \ . \tag{272}$$

Γ is a measure of the spread in energies of the distribution (270), and for that reason is called the *width* of the decaying state. Thus we see that the time-energy uncertainty relation is obeyed by the exponential decay law.

It should be noted that the exponential law is not a rigorous consequence of the distribution (270), and it is generally true that for times very short and very long compared to the lifetime there are departures from exponential decay. However, in the very important phenomena where the lifetime is far longer than the characteristic periods of the decaying system, such as beta decay or the radiative decay of excited states, the corrections to exponential decay are usually far too small to be observed.

(e) The Interaction Picture

Because the evolution of a system can be described either with stationary observables and moving state vectors, or the other way around, it is clear that descriptions in which both move are also available. Consider the case of a system whose Hamiltonian has the form $H_0 + V$, where both operators are time-independent, and H_0 is simple enough so that the time evolution it alone generates is known, but not that of the full Hamiltonian. An important example is scattering, with H_0 being the Hamiltonian of the free projectile and target, and V the interaction between them, without which there is no scattering. In this case the initial state, well before the collision, is a solution of the Schrödinger equation governed by H_0, but once the two objects come within range the evolution of the state is governed by $H_0 + V$. It can then be useful to remove the "trivial" time dependence due to H_0. The description that does this is called the *interaction picture.*

Let $|\psi;t\rangle_S$ be a state in the Schrödinger picture. Its counterpart in the interaction picture is then

$$|\psi;t\rangle_I = e^{iH_0 t/\hbar}|\psi;t\rangle_S \ ; \tag{273}$$

were there no interaction V, the left-hand side would be time-independent, i.e., in the Heisenberg picture. To obtain the equation of motion for $|\psi;t\rangle_I$, one substitutes $|\psi;t\rangle_S$ from (273) into the Schrödinger equation, and multiplies from the left by $e^{iH_0 t/\hbar}$:

$$e^{iH_0 t/\hbar}\,(i\hbar\partial_t - H_0 - V)\,e^{-iH_0 t/\hbar}\,|\psi;t\rangle_I = 0 \ . \tag{274}$$

This then yields the sought-for equation:

$$\left(i\hbar\frac{\partial}{\partial t} - V_I(t)\right)|\psi;t\rangle_I = 0 \ , \tag{275}$$

where

$$V_I(t) = e^{iH_0 t/\hbar}\, V\, e^{-iH_0 t/\hbar} \tag{276}$$

is V in the interaction picture.

We have already learned how, at least in principle, to find the time evolution when the Hamiltonian is time-dependent: namely, by solving Eq. 242. That is to say, in the interaction picture the movement of states is given by

$$|\psi; t\rangle_I = U_I(t, t')|\psi; t'\rangle_I \ , \tag{277}$$

where U_I is the solution of

$$\left(i\hbar\frac{\partial}{\partial t} - V_I(t)\right) U_I(t, t') = 0 \ , \tag{278}$$

with the initial condition $U_I(t, t) = 1$. This equation can only be solved directly if $[V_I(t), V_I(t')] = 0$ when $t \neq t'$. In this case, $V_I(t)$ is in effect a c-number, and

$$U_I(t, t') = \exp\left(-\frac{i}{\hbar}\int_{t'}^{t} d\tau\ V_I(\tau)\right) \ . \tag{279}$$

A complete solution is also known if the commutator $[V_I(t),\ V_I(t')]$ is a c-number.[1] In all but such exceptional cases, indeed, in almost all situations of real interest, no closed form solution is known. On the other hand, the solution in powers of V has been of enormous value. It is most easily derived form the integral equation that contains both the differential equation (278) and the initial condition:

$$U_I(t, t') = 1 - \frac{i}{\hbar}\int_{t'}^{t} d\tau\ V_I(\tau)\, U_I(\tau, t') \ . \tag{280}$$

By iteration this gives the Dyson expansion for the time evolution in the interaction picture:

$$U_I(t, t') = 1 - \frac{i}{\hbar}\int_{t'}^{t} d\tau\ V_I(\tau) + \left(\frac{i}{\hbar}\right)^2 \int_{t'}^{t} d\tau \int_{t'}^{\tau} d\tau'\ V_I(\tau)\, V_I(\tau') + \cdots \ . \tag{281}$$

2.5 Symmetries and Conservation Laws

Symmetries and conservation laws have a familiar relationship in classical physics. For a system whose Hamiltonian is invariant under both spatial translations and rotations, the linear and angular momenta are all constants of motion. This connection holds also in quantum mechanics, as will be shown shortly, though it has a somewhat different meaning because these six constants of motion do not all commute with each other. The other symmetry that plays a major role in classical physics concerns the relationship between inertial frames in relative motion, implemented by Galileo or Lorentz transformations, which are taken up in §7.3 and 13.2.

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[1] J. Schwinger, *Phys. Rev.* **75**, 651 (1949).

The symmetries just mentioned are continuous. The discrete symmetries of space reflection and time reversal are also important in classical mechanics and electrodynamics, but in quantum mechanics their implications are stronger. Finally, while it is a common thing in classical mechanics to consider systems of particles that have identical masses and other attributes, their indistinguishability has no particular consequence in the classical framework, whereas in quantum mechanics indistinguishability has enormous ramifications, as we will learn in chapters 6 and 12.

(a) Symmetries and Unitary Transformations

It is important to have a clear understanding of what is, and is not, meant by a symmetry. Let F and F' be two inertial frames related by one or more of the following: a translation in space or time, a spatial rotation, a uniform relative motion, a reflection in space, a reversal in time. Consider a system S prepared in arbitrary states $|\Psi_\alpha\rangle, |\Psi_\beta\rangle, \ldots$ to certain specifications by observables attached to F, and the states $|\Psi'_\alpha\rangle, |\Psi'_\beta\rangle, \ldots$ of S satisfying precisely the same specifications by observables attached to F'. On the assumption that these frames are equivalent, all the probabilities relating the states prepared in F must be equal to the corresponding relations in F':

$$|\langle\Psi_\alpha|\Psi_\beta\rangle|^2 = |\langle\Psi'_\alpha|\Psi'_\beta\rangle|^2 \ . \tag{282}$$

Were this not so, the probabilities could be used to distinguish between F and F'.

To carry this home, think of (282) as it applies to a one particle system, a state $|\Psi_{\boldsymbol{p}}\rangle$ of momentum $\boldsymbol{p}$ along the x-axis of F, another state $|\Psi_{lm}\rangle$ of total angular momentum l and projection m along the z-axis of F, the probability $|\langle\Psi_{\boldsymbol{p}}|\Psi_{lm}\rangle|^2$, and of the states having exactly these properties but with respect to a frame F' which is obtained by a rotation about the y-axis of F.

Note that according to the definitions used in (282), the condition of S described by the state $|\Psi'_\alpha\rangle$ differs from the condition described by $|\Psi_\alpha\rangle$ in that in the former S has been *moved* in some manner with respect to the latter as seen from the frame F; this is called the *active description.* There is another, equivalent, way of describing the situation: leaving the object fixed and defining $|\Psi'_\alpha\rangle$ to be state of this fixed object as observed from F'; this is called the passive description. *In this book we always use the active description.*

We stress that (282) is not a statement about interactions or dynamics — only about the properties of space and time. Eq. 282 must hold whatever the forces internal to or acting on the system S may be.

The probabilities in (282) will be equal if the corresponding probability amplitudes are equal apart from a phase factor,[1]

$$\langle\Psi_\alpha|\Psi_\beta\rangle = e^{i\lambda}\langle\Psi'_\alpha|\Psi'_\beta\rangle \ . \tag{283}$$

The indifference of the physical consequences to the phase factor is a restatement of the fact that quantum mechanics lives, so to say, in a ray space and not a Hilbert space. If the physically relevant space were a Hilbert space, and an arbitrary phase were inadmissible, then demanding that (282) hold for all Hilbert space vectors would require the kets $|\Psi'_\alpha\rangle$ to be related to the kets $|\Psi_\alpha\rangle$ by a *unitary* transfor-

[1] The case of time reversal is more complicated; see §7.2.

mation, for it is unitary transformations that leave scalar products invariant in complex vector spaces.

One might well fear that the admissibility of the phase factor would greatly complicate matters, but that is not so. The previously mentioned theorem due to Wigner states that there is just one physically important symmetry, time reversal, that cannot be implemented with a unitary transformation. Until chapter 7 we will, therefore, always resort directly to unitary transformations without mentioning these complications.

(b) Spatial Translations

Spatial translations were discussed in §2.3(a), but they merit a closer look because, while being especially simple, they introduce concepts that are important in more complicated symmetries.

Recall, first, that the unitary operator for a spatial translation $\boldsymbol{a}$ is

$$T(\boldsymbol{a}) = e^{-i\boldsymbol{P}\cdot\boldsymbol{a}/\hbar} \,, \tag{284}$$

where $\boldsymbol{P}$ is the total momentum operator for the system in question, and $\boldsymbol{a}$ is a numerical 3-vector. From geometry we know that spatial translations along different directions commute with each other, and therefore we demand that

$$[P_i, P_j] = 0 \,. \tag{285}$$

Let $\boldsymbol{x}_n$ be the coordinate operator of particle n. By its very definition, a coordinate operator must have the following behavior under translation:

$$T^\dagger(\boldsymbol{a})\boldsymbol{x}_n T(\boldsymbol{a}) = \boldsymbol{x}_n + \boldsymbol{a} \,. \tag{286}$$

If $|\psi\rangle$ is any state, then

$$T(\boldsymbol{a})|\psi\rangle = |\psi;\ \boldsymbol{a}\rangle \tag{287}$$

is that state displaced through the distance $\boldsymbol{a}$. (In this connection, recall Eq. 167 and Eq. 168.)

The eigenvalues of $\boldsymbol{x}_n$ will, as before, be called $\boldsymbol{r}_n$. Then the coordinate eigenkets are transformed as follows:

$$T(\boldsymbol{a})|\boldsymbol{r}_1, \ldots\rangle = |\boldsymbol{r}_n + \boldsymbol{a}, \ldots\rangle \,, \quad T^\dagger(\boldsymbol{a})|\boldsymbol{r}_1, \ldots\rangle = |\boldsymbol{r}_n - \boldsymbol{a}, \ldots\rangle \,. \tag{288}$$

The original and spatially transformed wave function are, by definition,

$$\psi(\boldsymbol{r}_1, \ldots) = \langle \boldsymbol{r}_1, \ldots|\psi\rangle \,, \qquad \psi'(\boldsymbol{r}_1, \ldots) = \langle \boldsymbol{r}_1, \ldots|T(\boldsymbol{a})|\psi\rangle \tag{289}$$

Hence

$$\psi'(\boldsymbol{r}_1 \ldots) = \psi(\boldsymbol{r}_1 - \boldsymbol{a}, \ldots) \,. \tag{290}$$

Note carefully that the coordinates on the right-hand side of this relationship have been translated in the direction opposite to that of the state $|\psi\rangle$. Furthermore, from $T^\dagger T = 1$ it follows immediately that

$$\psi'(\boldsymbol{r}_1 + \boldsymbol{a} \ldots) = \psi(\boldsymbol{r}_1 \ldots) \,. \tag{291}$$

Equations (291) and (290) are special cases of general results that holds for all unitary transformation. Namely, if P' is the image of the point P under any transformation τ, i.e., if $P' = \tau P$, and $|\psi\rangle$ and $|\psi'\rangle$ any state and its image under τ produced by the unitary operator $U(\tau)$, then the transformation laws for wave functions are

$$\psi'(P') = \psi(P) \,, \tag{292}$$

and

$$\psi'(P) = \psi(\tau^{-1}P) \,. \tag{293}$$

The geometrical explanation for this important and generic fact is illustrated below for the case of rotations. Now let $F(\boldsymbol{x}_n)$ be any observable constructed from coordinates. Then

$$T^\dagger(\boldsymbol{a})F(\boldsymbol{x}_n)T(\boldsymbol{a}) = F(\boldsymbol{x}_n + \boldsymbol{a}) \,. \tag{294}$$

In particular, for an infinitesimal translation,

$$F(\boldsymbol{x}_n + \delta\boldsymbol{a}) = F(\boldsymbol{x}_n) + \frac{i}{\hbar}\sum_i \delta a_i [P_i, F(\boldsymbol{x}_n)] \,. \tag{295}$$

Hence if a function of the coordinates is invariant under a translation along the ith direction, it commutes with that component of the total momentum.

The connection between the momentum conservation law and invariance under spatial translation now follows in close analogy to that of classical mechanics. Namely, *if the Hamiltonian is invariant under spatial translations, the total momentum commutes with the Hamiltonian and is therefore a constant of motion.* The last part of this statement is a special case of the general theorem that observables that commute with H are constants of motion. Equation (294) also tells us that if H is only invariant under translations along one direction (or in one plane), only the momentum along that direction (or in that plane) is a constant of motion.

(c) Symmetry Groups

By considering a sequence of translations, one is led quite naturally to the concept of a group of symmetries. Take the translation through $\boldsymbol{a}$ followed by $\boldsymbol{b}$:

$$T(\boldsymbol{b})T(\boldsymbol{a}) = T(\boldsymbol{a} + \boldsymbol{b}) \,. \tag{296}$$

Because the argument of the composite translation is the sum of $\boldsymbol{a}$ and $\boldsymbol{b}$, the order in which these translations are carried out does not matter; they commute. Of course, we already knew that because the various components of $\boldsymbol{P}$ commute with each other, but this tells us that $[P_i, P_j] = 0$ is a requirement set by Euclidean geometry itself, not dynamics. The special case $\boldsymbol{b} = -\boldsymbol{a}$, which just undoes the first translation, is also of interest:

$$T(\boldsymbol{a})T(-\boldsymbol{a}) = T(\boldsymbol{a})T^\dagger(\boldsymbol{a}) = T(0) = 1 \,, \tag{297}$$

where 1 expresses the fact that no change is produced.

The relations (296) and (297) show that *the operators $T(\boldsymbol{a})$ form an Abelian Lie group of unitary operators standing in one-to-one correspondence with the group of translation in the Euclidean 3-space* $\mathfrak{E}_3$.

This wallop of jargon will now be explained because it plays so large a role in the discussion of symmetries in quantum mechanics.

- A group $\mathfrak{G}$ is a finite or infinite set of elements $(g_1, g_2, \ldots)$ having a composition law for every pair of elements such that $g_1 g_2$ is again an element of $\mathfrak{G}$; which is associative, i.e., $(g_1 g_2)g_3 = g_1(g_2 g_3)$; and with every element g_i having an inverse g_i^{-1} such that $g_i g_i^{-1}$ is the identity element I, i.e., $Ig_i = g_i I = g_i$ for all i.

- A group is Abelian if all its elements commute, i.e., $g_1 g_2 = g_2 g_1$.

- A group with an infinite set of elements is a Lie group if its elements can be uniquely specified by a set of *continuous* parameters $(z_1 \ldots z_r)$.

Two distinct but closely related groups are in play in the case of translations: both are Abelian Lie groups, parametrized by the components of a 3-vector $\boldsymbol{a}$. One is the group of translations in every-day Euclidean 3-space, $\mathfrak{E}_3$; it is Abelian because translations along different directions commute. The second is a group of unitary operators in Hilbert space; it is Abelian because the components of the total momentum $\boldsymbol{P}$ operator commute with each other. Their one-to-one correspondence is implemented by giving the elements of both groups the same parametrization and the same composition laws.

It would, therefore, be natural to say that the unitary operators T form a representation of the translation group in Hilbert space. But the term "representation" is, by tradition, reserved for matrices whose multiplication law stands in one-to-one correspondence with the algebra of the group. That is, if $\{|\xi\rangle\}$ is any basis in $\mathfrak{H}$, the matrices with elements $\langle\xi|T|\xi'\rangle$ form a representation of this group in that

$$\sum_{\xi''} \langle\xi|T(\boldsymbol{a})|\xi''\rangle\langle\xi''|T(\boldsymbol{b})|\xi'\rangle = \langle\xi|T(\boldsymbol{a}+\boldsymbol{b})|\xi'\rangle \,, \tag{298}$$

which is true by virtue of (296).

In equating sequences of transformation to products of unitary transformations, as we have done starting with (296), we have ignored the fact that multiplying the product by an arbitrary phase would not have any physical consequence because physical states are rays and not vectors. That is to say, if τ_i stands for the parameters specifying some particular transformation (such as $\boldsymbol{a}$ in the case of a translation), $\tau_2\tau_1$ for the parameters that specify the indicated sequence of transformations, and $U(\tau_i)$ the corresponding unitary operators, then in contrast to (296) or (298), we are free to write

$$U(\tau_2)U(\tau_1) = e^{i\lambda}\, U(\tau_2\tau_1) \,. \tag{299}$$

Once again, one could worry that ignoring the phase factor is illegitimate. However, it is only for Galileo transformations that this issue matters, as we shall see in §7.3; in all other cases the phases of the states can be chosen so that there is no phase factor in the product of unitary transformations.

Next, consider the generalization of the infinitesimal translation $\delta\boldsymbol{a}$,

$$T = 1 - i\delta\boldsymbol{a}\cdot\boldsymbol{P}/\hbar \,. \tag{300}$$

Quite generally, if a unitary operator $U(z_1 \ldots z_r)$ carries out a transformation belonging to a Lie group, then if the transformation is infinitesimal it has the form

$$U = 1 - i\sum_{l=1}^{r} \delta z_l\, \mathcal{G}_l \,, \tag{301}$$

where the operators $\mathcal{G}_l$, which must be Hermitian for U to be unitary, are called the *generators* of the group $\mathfrak{G}$. In the case of the spatial translation group, the generators are the three components of the total momentum $\boldsymbol{P}$ (for convenience divided by $\hbar$ to give them the dimension of momentum). The algebra obeyed by the generators as defined by their commutators is called the *Lie algebra* of $\mathfrak{G}$. It is called Abelian if the generators commute, as they do for the translation group.

Because it is just Euclidean geometry that defines the properties of the translation group, the Lie algebra associated with this group cannot depend on quantum mechanics for its construction. To see this, let $f(x_1x_2x_3)$ be any function of the coordinates in $\mathfrak{E}_3$, taken now to be real numbers and not operators, and consider the infinitesimal translation $x_i \to x_i + \delta a_i$. Then

$$\delta f = f(x_i + \delta a_i) - f(x_i) = \sum_i \delta a_i \frac{\partial f}{\partial x_i} \; ; \tag{302}$$

in this formulation the differential operators $\partial/\partial x_i$ are the commuting infinitesimal generators. Putting this into the form

$$\delta f = \frac{i}{\hbar} \sum_i \delta a_i \frac{\hbar}{i} \frac{\partial f}{x_i} \; , \tag{303}$$

shows how the momentum in the Schrödinger representation is related to translation in space.

Equation (302) is actually (295) in another guise, which can be seen by recalling Eq. 162 rewritten in the notation being used here:

$$[\boldsymbol{p}_n, F(\boldsymbol{x}_1 \ldots \boldsymbol{x}_N)] = \frac{\hbar}{i} \frac{\partial F}{\partial \boldsymbol{x}_n} \; , \qquad [\boldsymbol{x}_n, G(\boldsymbol{p}_1 \ldots \boldsymbol{p}_N)] = i\hbar \frac{\partial G}{\partial \boldsymbol{p}_n} \; ; \tag{304}$$

thus

$$\delta F = \sum_n \delta \boldsymbol{a} \cdot \frac{\partial F}{\partial \boldsymbol{x}_n} = \frac{i}{\hbar} \sum_n [\delta \boldsymbol{a} \cdot \boldsymbol{p}_n, F] \, , \tag{305}$$

which is (295).

If the Lie algebra is non-Abelian, it is not straightforward to construct the unitary transformations for finite values of all the parameters. However, for the *subgroup* defined by setting all but one parameter, which we call z, to zero, it is straightforward to construct a finite transformation because only one generator, $\mathcal{G}$, is involved, so that it behaves like a number as nothing with which it does not commute is involved. Then the argument that led to the time translation operator (Eq. 213) carries through as it stands, and so for this subgroup

$$U(z) = e^{-iz\mathcal{G}} \, . \tag{306}$$

(d) Rotations

Many of the systems of interest in quantum mechanics are either exactly or approximately invariant under rotations. However, rotations about different axes do not commute, and therefore the rotation group is non-Abelian, which makes its analysis quite complicated. For these reasons a significant portion of this volume will be devoted to developing this analysis and applying it to various physical problems.

The parametrization of rotations in $\mathfrak{E}_3$ can be done in a variety of ways. Here we will specify a rotation R by the unit vector $\boldsymbol{n}$ along an axis of rotation, and an angle of rotation θ about that axis, with the convention that the rotation is counterclockwise when looking along $\boldsymbol{n}$ towards the origin, and $0 \leq \theta \leq 2\pi$.

As with translations, a great deal can be learned from infinitesimal transformations. An infinitesimal rotation will be parametrized by

$$\delta\boldsymbol{\omega} = \boldsymbol{n}\,\delta\theta\ . \tag{307}$$

Under this rotation, a vector $\boldsymbol{K}$ in $\mathfrak{E}_3$ transforms as follows:

$$\boldsymbol{K} \to \boldsymbol{K} + \delta\boldsymbol{\omega}\times\boldsymbol{K} \equiv \boldsymbol{K} + \delta\boldsymbol{K}\ , \tag{308}$$

or in terms of Cartesian components,

$$\delta K_i = \epsilon_{ijk}\delta\omega_j K_k\ , \tag{309}$$

where ϵ_{ijk} is the totally antisymmetric Levi-Civita tensor, with $\epsilon_{123} = 1$.

If $\boldsymbol{K}$ is written as a column 3-vector, rotations through any angle can be carried out with the help of the following 3×3 matrices:

$$I_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}\ , \quad I_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}\ , \quad I_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{310}$$

A finite rotation of $\boldsymbol{K}$ about a single axis, say, about the axis 1 through the angle ϕ_1, is accomplished by

$$\boldsymbol{K} \to \boldsymbol{K}' = e^{-i\phi_1 I_1}\,\boldsymbol{K}\ . \tag{311}$$

Successive rotations of $\boldsymbol{K}$ about distinct axes do not commute, a fact that is captured in the commutation rule

$$[I_i, I_j] = i\epsilon_{ijk}\,I_k\ . \tag{312}$$

Quantum mechanics enters by assigning, to every rotation R in $\mathfrak{E}_3$, a unitary transformation $D(R)$ on the Hilbert space $\mathfrak{H}$ of the system of interest. To be concrete, one can think of $\boldsymbol{K}$ as a vector in everyday $\mathfrak{E}_3$ that identifies some point in an apparatus that is used to prepare or measure states of the system. Consistency requires the correspondence between rotations in $\mathfrak{E}_3$ and the unitary transformations in $\mathfrak{H}$ to be maintained when two (or more) rotations are carried out in succession. Let R_2R_1 be the rotation in $\mathfrak{E}_3$ that results from carrying out R_1 followed by R_2. The consistency requirement is then

$$D(R_2R_1) = D(R_2)\,D(R_1)\ . \tag{313}$$

As rotations in $\mathfrak{E}_3$ do not commute, it is clear that in general

$$D(R_1)D(R_2) \neq D(R_2)D(R_1)\ . \tag{314}$$

The exception is the set of successive rotations about one, and only one axis $\boldsymbol{n}$. The argument that led to the general result (306) implies that such rotations can be written in the form

$$D(R) = \exp(-i\theta\boldsymbol{n}\cdot\boldsymbol{J})\ , \tag{315}$$

where the Hermitian generator $\boldsymbol{n}\cdot\boldsymbol{J}$ is, by definition, *the component of angular momentum along the direction* $\boldsymbol{n}$.

The implications of the requirement (313) emerge from considering two successive infinitesimal rotations about two distinct axes, say, through $(\delta\phi_1,\ \delta\phi_2)$ about the axes 1 and 2, in both possible orders:

$$\boldsymbol{K}' = (1 - i\delta\phi_2 I_2 + \ldots)(1 - i\delta\phi_1 I_1 + \ldots)\,\boldsymbol{K}\ , \tag{316}$$

$$\boldsymbol{K}'' = (1 - i\delta\phi_1 I_1 + \ldots)(1 - i\delta\phi_2 I_2 + \ldots)\,\boldsymbol{K}\ . \tag{317}$$

These two rotated vectors are not identical:[1]

$$\boldsymbol{K}'' - \boldsymbol{K}' = \{-\delta\phi_1\delta\phi_2(I_1I_2 - I_2I_1) + \ldots\}\boldsymbol{K} = \{-i\delta\phi_1\delta\phi_2\, I_3 + O(\delta\phi^3)\}\boldsymbol{K}\ . \tag{318}$$

The correspondence to the unitary operators $D(R)$ must maintain this difference. In view of (315), they must thus satisfy

$$\lim_{\delta\phi_i\to 0}\left(e^{-i\delta\phi_1 J_1}\,e^{-i\delta\phi_2 J_2} - e^{-i\delta\phi_2 J_2}\,e^{-i\delta\phi_1 J_1}\right) = -i\delta\phi_1\delta\phi_2\, J_3 + O(\delta\phi^3)\ . \tag{319}$$

Hence $[J_1, J_2] = iJ_3$, and in general,

$$[J_i, J_j] = i\epsilon_{ijk}\, J_k\ . \tag{320}$$

This is *the angular momentum commutation rule.*

This derivation of the angular momentum commutation rule relied on no assumption concerning the dynamical variables of some system.[2] It therefore applies to all systems, whether they be composed of structureless particles with no internal degrees of freedom; or particles that have an intrinsic angular momentum, or spin, which is not a function of canonical coordinates and momenta; or the quantized electromagnetic field. Whatever the system may be, we have been speaking of rotating the system as a whole, and $\boldsymbol{J}$ is therefore the system's total angular momentum. (One can, of course, imagine rotations of some component of a system, and the same geometrical argument will then lead to the same commutation rule for the angular momentum of that component.)

Let A be any observable. Under the rotation R it undergoes the unitary transformation

$$A \to D^\dagger(R)\, A\, D(R)\ . \tag{321}$$

If R is infinitesimal,

$$A \to A + \delta A\ , \qquad \delta A = i\delta\theta\,[\boldsymbol{n}\cdot\boldsymbol{J}, A]\ . \tag{322}$$

Hence if an observable is invariant under rotations about $\boldsymbol{n}$*, it commutes with the corresponding component of angular momentum.* An observable that is invariant under rotations about all directions is called a *scalar* under rotations.

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[1] The generalization of this result to arbitrary infinitesimal rotations is the subject of Prob. 10.

[2] While (320) follows from (312) by $I_i \to J_i$, this is only a mnemonic; I_i is a 3×3 matrix acting on garden variety 3-vectors whereas J_i is an operator in a Hilbert space that is only specified when the system in question is identified. As we shall see in §3.3, the I_i are the angular momentum operators in the 3-dimensional (or $j = 1$) representation, though not in the conventional form in which the 3-component is diagonal.

The angular momentum conservation law now follows as it does for linear momentum: *If the Hamiltonian is invariant under rotations about an axis, the component of the total angular momentum along that axis is a constant of motion.*

All sorts of quantities that are not scalars play important roles in physics. A general classification of non-invariant observables will be given in §7.6; here we only treat the most important and simplest class — *vector operators.* By definition, a set of three observables $(V_1, V_2, V_3) = \boldsymbol{V}$ is called a vector operator if it transforms under rotations in the same way as does the c-number vector $\boldsymbol{K}$ in (308):

$$\delta \boldsymbol{V} = i\delta\theta\,[\boldsymbol{n}\cdot\boldsymbol{J}, \boldsymbol{V}] = \delta\theta\,\boldsymbol{n}\times\boldsymbol{V}\ . \tag{323}$$

In short, the definitions (308) and (323) are completely general — whether the vector is the line from this word to your nose, or the momentum operator of a neutron in some nucleus. Or put another way, anything that transforms in this way *is* a vector.

The coefficients of n_i in (323) must be equal, and $\boldsymbol{V}$ must therefore obey the commutation rule[1]

$$[V_i, J_j] = i\epsilon_{ijk}\,V_k\ . \tag{324}$$

Any set of three observables that satisfy this commutation rule with the angular momentum constitute a vector operator. In particular, the angular momentum $\boldsymbol{J}$ is itself a vector operator, as comparison of (324) to (320) shows, and common sense requires.

It is instructive to verify that the unitary transformation (321) does properly transform a vector operator under finite rotations. For this purpose it suffices to consider a rotation about any one axis. Define

$$V_i(\theta) = e^{i\theta J_3} V_i e^{-i\theta J_3}\ . \tag{325}$$

Then

$$\frac{dV_i(\theta)}{d\theta} \equiv \dot{V}(\theta) = ie^{i\theta J_3}[J_3, V_i]e^{-i\theta J_3}\ , \tag{326}$$

so $\dot{V}_1 = -V_2, \dot{V}_2 = V_1, \dot{V}_3 = 0$. Therefore $\ddot{V}_i = -V_i$ for $i = 1, 2$, which after integration gives the proper answer:

$$e^{i\theta J_3} V_1 e^{-i\theta J_3} = V_1\cos\theta - V_2\sin\theta\ , \quad e^{i\theta J_3} V_2 e^{-i\theta J_3} = V_2\cos\theta + V_1\sin\theta\ . \tag{327}$$

The total momentum $\boldsymbol{P}$ of a system, being a vector, does not commute with the total angular momentum; only components of $\boldsymbol{P}$ and $\boldsymbol{J}$ along the same direction commute.

The scalar product of two vector operators is invariant under rotation, and must therefore commute with $\boldsymbol{J}$, as is easily confirmed by applying (324) to $\boldsymbol{V}_1\cdot\boldsymbol{V}_2$. In particular, therefore, J^2 and P^2 both commute with $\boldsymbol{J}$, and also each other.

While all components of $\boldsymbol{P}$ and $\boldsymbol{J}$ are constants of motion if the Hamiltonian is invariant under translations and rotations, they cannot all be diagonalized simultaneously. Hence it is not possible to construct simultaneous eigenstates of all these six constants of motion. In addition to the rotational scalars P^2, J^2 and $\boldsymbol{P}\cdot\boldsymbol{J}$, one component of angular momentum, traditionally defined to be J_3, can be diagonalized simultaneously, and states can be designated by the associated eigenvalues.

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[1] In the older literature this commutation rule is often written as $\boldsymbol{V}\times\boldsymbol{J} = i\boldsymbol{V}$.

As an illustration of this totally general discussion, consider a single particle with position and momentum operators $\boldsymbol{x}$ and $\boldsymbol{p}$. The *orbital angular momentum operator* $\boldsymbol{L}$ for this particle is then defined as

$$\boldsymbol{L} = (\boldsymbol{x}\times\boldsymbol{p})/\hbar\,, \tag{328}$$

or

$$L_i = \epsilon_{ijk} x_j p_k/\hbar\,. \tag{329}$$

The factor $1/\hbar$ in the definition of $\boldsymbol{L}$, and the absence of $\hbar$ in (320), have the consequence that *all angular momenta are dimensionless*, a convention that will be adhered to throughout. It should also be mentioned that the order of x_j and p_k in (329) does not matter because only commuting factors appear in L_i.

The commutation rule for the orbital angular momentum now follow from (329) when the canonical commutation rule $[x_i, p_j] = i\delta_{ij}\hbar$ is used:

$$[L_i, L_j] = i\epsilon_{ijk}\, L_k\,. \tag{330}$$

That this is identical in form to the general rule (320) is simply a consequence of the requirement that the rotations in $\mathfrak{E}_3$ are to be translated into unitary operators in one and the same way no matter what the system may be. Furthermore, from the canonical commutation rules

$$[x_i, L_j] = i\epsilon_{ijk}\, x_k\,, \qquad [p_i, L_j] = i\epsilon_{ijk}\, p_k\,. \tag{331}$$

Hence $\boldsymbol{x}$ and $\boldsymbol{p}$ are vector operators, again as common sense requires.

The role of the orbital angular momentum operator in rotations can also be seen in a slightly different light as follows. Let $\psi(\boldsymbol{r})$ be some wave function, where $\boldsymbol{r} = (r_1, r_2, r_3)$ is the eigenvalue of $\boldsymbol{x}$. Under a infinitesimal rotation about $\boldsymbol{n} = (0, 0, 1)$, the change in ψ is

$$\begin{aligned}\delta\psi(\boldsymbol{r}) &= \psi(r_1 - r_2\delta\theta, r_2 + r_1\delta\theta, r_3) - \psi(r_1, r_2, r_3)\\ &= -\delta\theta\left(r_2\frac{\partial}{\partial r_1} - r_1\frac{\partial}{\partial r_2}\right)\psi(\boldsymbol{r})\\ &= \delta\theta\frac{i}{\hbar}(x_1p_2 - x_2p_1)\psi(\boldsymbol{r}) = i\delta\theta\, L_3\,\psi(\boldsymbol{r})\,,\end{aligned} \tag{332}$$

where in the last expressions the p_i and L_i have become differential operators. This too is required by consistency, because under a rotation R, the state $|\psi\rangle$ and the eigenket $|\boldsymbol{r}\rangle$ of $\boldsymbol{x}$ undergo the transformations

$$|\psi\rangle \to D(R)|\psi\rangle \equiv |\psi'\rangle\,, \qquad |\boldsymbol{r}\rangle \to D(R)|\boldsymbol{r}\rangle = |R\boldsymbol{r}\rangle\,, \tag{333}$$

where $R\boldsymbol{r}$ is the rotated image of $\boldsymbol{r}$. The wave function therefore transforms as follows:

$$\langle\boldsymbol{r}|\psi\rangle \to \langle\boldsymbol{r}|D(R)|\psi\rangle = \langle R^{-1}\boldsymbol{r}|\psi\rangle\,, \tag{334}$$

and therefore

$$\psi'(\boldsymbol{r}) = \psi(R^{-1}\boldsymbol{r})\,. \tag{335}$$

This illustrates the general relationship Eq. 293.

When R is the infinitesimal rotation of (332), this last equation becomes

$$\psi(\boldsymbol{r}) \to \psi'(\boldsymbol{r}) = (1 + i\delta\theta L_3)\,\psi(\boldsymbol{r})\,, \tag{336}$$

where L_3 is again the differential representation of the operator. The sign difference between (336) and $D = 1 - i\delta\theta L_3$ results from the fact that when an object (here the state $|\psi\rangle$) is rotated through R, the point that is then on the object at $\boldsymbol{r}$ was originally located at $R^{-1}\boldsymbol{r}$ in the fixed coordinate frame (see Fig. 2.3). Note that this last statement, and our whole treatment of rotations, has been in the active mode.

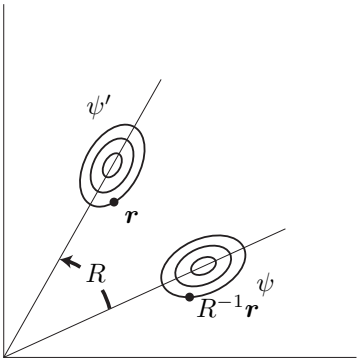

FIG. 2.3. The relationship between rotated states (Eq. 334) as an example of the general case (Eq. 293). The curves are contours of ψ = const.

(e) Space Reflection and Parity

Vectors that change sign under a reflection through the origin are called *polar vectors,* and those that do not change sign are called *axial vectors.* Coordinates, momenta and electric fields $\boldsymbol{E}$ are polar vectors, whereas angular momenta and magnetic fields $\boldsymbol{B}$ are axial vectors. A quantity like $\boldsymbol{E}\cdot\boldsymbol{B}$, which is invariant under rotations but changes sign under reflection, is called a *pseudoscalar.* It is sometimes convenient to reflect through a plane instead of the origin, but there is no fundamental distinction between these as they are related by a rotation of π about the normal to the reflection plane. Unless stated otherwise, the term "reflection" will mean through the origin.

Space reflection is implemented by a unitary operator I_s. By definition, it has the following effect on positions and momenta:[1]

$$I_s^\dagger \boldsymbol{x}_n I_s = -\boldsymbol{x}_n, \qquad I_s^\dagger \boldsymbol{p}_n I_s = -\boldsymbol{p}_n\,, \tag{337}$$

and therefore the opposite effect on angular momenta:

$$I_s^\dagger \boldsymbol{J} I_s = \boldsymbol{J}\,. \tag{338}$$

[1]The canonical commutation rule is, therefore, invariant under space reflection. Time reversal only changes the sign of $\boldsymbol{p}$, but not of $\boldsymbol{x}$, and therefore it would *not* leave the canonical commutation rule invariant if it were implemented by a unitary transformation. For this, and other related reasons, a non-unitary transformation is involved in time reversal, as will be discussed in §7.2.

Let $|\psi\rangle$ be some state. It may or may not be an eigenstate of I_s. However, if it is, and has eigenvalue i_s, i.e., if

$$I_s|\psi\rangle = i_s|\psi\rangle \ , \tag{339}$$

then because $(I_s)^2 = 1$, it follows that

$$i_s = \pm 1 \ . \tag{340}$$

This eigenvalue (or quantum number) is called the *parity.* It has no counterpart in classical mechanics, but plays a crucial role in quantum mechanics.

If the Hamiltonian is invariant under reflection, parity is a constant of motion and energy eigenstates can be assigned a definite parity — even or odd. The words "can be" appear here because it does happen (e.g., in hydrogen!) that even though the Hamiltonian is reflection invariant energy eigenstates of different parity are degenerate, and when that is so linear combinations of states of differing parity are also energy eigenstates.

Linear and angular momentum are *additive constants of motion.* This statement has the following simple meaning: If $\{S_i\}$ is a set of N non-interacting systems, then this set has states of the form

$$|\Psi\rangle = |\psi(S_1)\rangle \otimes \ldots \otimes |\psi(S_N)\rangle \, , \tag{341}$$

and if $|\psi(S_i)\rangle$ are eigenstates of, say, momentum with eigenvalue $\boldsymbol{P}_i$, then $|\Psi\rangle$ is an eigenstate of momentum with an eigenvalue that is the sum of those of the constituents. This statement holds also for any one component of angular momentum, and for the energy.

By contrast, *parity is a multiplicative quantum number.* For the state defined in (341), in an obvious notation

$$i_s = \prod_k i_s(S_k) \ . \tag{342}$$

(f) Gauge Invariance

Gauge invariance is a symmetry that arises in classical electrodynamics, but it has flowered into a theme of central importance in the generalizations of electrodynamics to the other fundamental interactions of physics.

In electrodynamics it is often advantageous to replace the electric and magnetic field strengths by the scalar and vector potentials $\phi(\boldsymbol{r}, t)$ and $\boldsymbol{A}(\boldsymbol{r}, t)$:

$$\boldsymbol{E}(\boldsymbol{r}, t) = -\boldsymbol{\nabla}\phi(\boldsymbol{r}, t) - \frac{1}{c}\frac{\partial}{\partial t}\,\boldsymbol{A}(\boldsymbol{r}, t) \ , \tag{343}$$

$$\boldsymbol{B}(\boldsymbol{r}, t) = \boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{r}, t) \ . \tag{344}$$

The field strengths are left invariant under the gauge transformation

$$\boldsymbol{A}(\boldsymbol{r}, t) \to \boldsymbol{A}'(\boldsymbol{r}, t) = \boldsymbol{A}(\boldsymbol{r}, t) + \boldsymbol{\nabla}\chi(\boldsymbol{r}, t) \ , \tag{345}$$

$$\phi(\boldsymbol{r}, t) \to \phi'(\boldsymbol{r}, t) = \phi(\boldsymbol{r}, t) - \frac{1}{c}\frac{\partial}{\partial t}\,\chi(\boldsymbol{r}, t) \ , \tag{346}$$

where $\chi(\boldsymbol{r},t)$ is an arbitrary (smooth) function. In short, the field strengths have an invariant physical meaning, whereas potentials that differ only by gauge transformations represent the same physical situation in classical physics.

The classical Hamiltonian for a system of charged particles is turned into the operator H in Schrödinger's equation by the standard recipe

$$\boldsymbol{p}_n \to \frac{\hbar}{i}\frac{\partial}{\partial \boldsymbol{r}_n} \ , \tag{347}$$

so that

$$H = \sum_{n=1}^{N} \left\{ \frac{1}{2m_n} \left(\frac{\hbar}{i}\frac{\partial}{\partial \boldsymbol{r}_n} - \frac{e_n}{c}\boldsymbol{A}(\boldsymbol{r}_n,t) \right)^2 + e_n\phi(\boldsymbol{r}_n,t) \right\} + V \ , \tag{348}$$

where V is the electrostatic energy due to the interaction between these particles, and $\phi(\boldsymbol{r},t)$ the potential describing the applied electric field. To make Schrödinger's equation invariant under the gauge transformation on the potentials, the wave function must also change to compensate. Because of the spatial derivatives in H, and the time derivative in Schrödinger's equation, this is accomplished by changing the phase of the wave function as follows:

$$\psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N,t) \to \psi'(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N,t) = \prod_{n=1}^{N} \exp\left(\frac{ie_n}{\hbar c}\,\chi(\boldsymbol{r}_n,t) \right)\ \psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N,t) \ . \tag{349}$$

In quantum mechanics, therefore, the term *gauge transformation* refers to the combined transformations on ϕ, $\boldsymbol{A}$ and ψ. There is a fundamental difference between classical and quantum physics, however: in the quantum case, the potentials themselves can be of physical significance in situations where the electromagnetic field is in a topologically non-trivial space, such as the region outside a tube (see §4.3(d)).

The change of phase (349) is a unitary transformation in the Hilbert space, but the change of the potentials, which are not operators here, is not a unitary transformation. Nevertheless, the gauge transformation form an Abelian group: two successive transformations are again a gauge transformation, their order does not matter, and every transformation has an inverse.

The operator

$$\boldsymbol{v}_n = \frac{1}{m_n}\left(\frac{\hbar}{i}\frac{\partial}{\partial \boldsymbol{r}_n} - \frac{e_n}{c}\boldsymbol{A}(\boldsymbol{r}_n,t) \right) \tag{350}$$

represents the velocity of particle n; this is confirmed by computing the time derivative of the coordinate operator. For that reason it is to be expected that the probability current is not (227) when the system interacts with an electromagnetic field, but is rather

$$\boldsymbol{i}_n(\boldsymbol{r}_1,\ldots;t) = \frac{1}{2}\left\{ \psi^*\boldsymbol{v}_n\psi + \psi(\boldsymbol{v}_n\psi)^* \right\} \ . \tag{351}$$

The probability density remains $|\psi|^2$. That (351) is correct is confirmed by showing that it satisfies the continuity equation (226) as a consequence of the Schrödinger equation when (348) is the Hamiltonian.

2.6 Propagators and Green's Functions

The two initial formulations of quantum mechanics, stemming from Heisenberg and Schrödinger, have now been described. The path integral, a later equivalent formulation due to Feynman, can be motivated by the insights revealed by the interference experiments discussed in chapter 1. For that reason, the path integral can be viewed as having a more intimate connection to the conceptual essentials of quantum mechanics. One can therefore take the position that quantum mechanics is defined by the path integral, which is how it was introduced originally by Feynman. We, however, will derive it from Schrödinger's equation in the following section. This section prepares the ground for this task, and in so doing it develops some powerful tools that are important in their own right.

The Schrödinger equation, like any linear partial differential equation, can be turned into an integral equation that states the boundary conditions up front. For the time-dependent equation, the kernel of the integral equation will be called the propagator, while for the time-independent equation it will be called Green's function. Readers should however note that many authors use the latter name for both. As is to be expected, these two kernels are each others Fourier transforms.

(a) Propagators

Schrödinger's differential equation is of first order in time, so an initial condition must be specified if it is to manufacture a definite solution. The initial condition can be made organic to the formulation if the differential equation is recast as an integral equation. For this purpose recall Eq. 207,

$$|\psi;t\rangle = U(t,t')|\psi;t'\rangle\,. \tag{352}$$

In terms of this unitary operator, the Schrödinger equation is

$$[i\hbar\partial_t - H(t)]U(t,t') = 0\,, \tag{353}$$

which holds also for a time-dependent Hamiltonian. Let $\boldsymbol{r} \equiv (\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)$ be a point in the configuration space $\mathfrak{C}$ of the system, and $|\boldsymbol{r}\rangle$ be a simultaneous eigenket of all the coordinate operators. Then

$$\psi(\boldsymbol{r};t) = \int d\boldsymbol{r}'\,\langle \boldsymbol{r}|U(t,t')|\boldsymbol{r}'\rangle\;\psi(\boldsymbol{r}';t')\,, \tag{354}$$

where $d\boldsymbol{r} \equiv d^3r_1\ldots d^3r_N$. This equation moves the state both into the future and the past.

An equation that singles out the future is obtained by introducing the *propagator* K, defined as the function

$$K(\boldsymbol{r}t,\boldsymbol{r}'t') = \langle \boldsymbol{r}|U(t,t')|\boldsymbol{r}'\rangle\,\theta(t-t')\,, \tag{355}$$

where $\theta(x)$ is the unit step (or Heaviside) function:

$$\theta(x) = \begin{cases} 1 & x>0 \\ 0 & x<0 \end{cases} \quad ; \qquad \frac{d}{dx}\theta(x) = \delta(x)\,. \tag{356}$$

Because $U(t,t') \to 1$ as $t \to t'$ from above,

$$\lim_{t\to t'} K(\boldsymbol{r}t, \boldsymbol{r}'t') = \delta(\boldsymbol{r}-\boldsymbol{r}') \,, \tag{357}$$

where the right-hand side is the $3N$-fold delta function.

As is clear from its definition, *the propagator is a probability amplitude — the amplitude for finding the system at some point* $\boldsymbol{r}$ *in configuration space at time* t *given that it was originally at* $\boldsymbol{r}'$ at time t'. For that reason the following notation is also often used:

$$K(\boldsymbol{r}t, \boldsymbol{r}'t') = \langle \boldsymbol{r}; t | \boldsymbol{r}'; t' \rangle \,, \qquad (t \geq t') \,. \tag{358}$$

The propagator satisfies an inhomogeneous counterpart of the Schrödinger equation:

$$[i\hbar\partial_t - H(t)] K(\boldsymbol{r}t, \boldsymbol{r}'t') = i\hbar\delta(t-t')\,\delta(\boldsymbol{r}-\boldsymbol{r}') \,, \tag{359}$$

where HK is shorthand for the operator H acting on the variables $\boldsymbol{r}$, e.g., by differentiation in the case of the kinetic energy. Equation (359) follows from (353), (355), and (356):

$$i\hbar\partial_t K(\boldsymbol{r}t; \boldsymbol{r}'t') = HK(\boldsymbol{r}t; \boldsymbol{r}'t') + \langle \boldsymbol{r}|U(t,t')|\boldsymbol{r}'\rangle \; i\hbar\delta(t-t') \,, \tag{360}$$

and $\delta(t-t')U(t,t') = \delta(t-t')$. As K satisfies the inhomogeneous equation (359) with a unit source, it is frequently called Green's function for the time-dependent Schrödinger equation, but to avoid confusion the term *Green's function* will be reserved here for a closely related time-independent object to be defined shortly.

The group property $U(t_3,t_2)U(t_2,t_1) = U(t_3,t_1)$ implies the following important composition law for the propagator:

$$K(\boldsymbol{r}t, \boldsymbol{r}t') = \int d\boldsymbol{r}''\, K(\boldsymbol{r}t, \boldsymbol{r}''t'')\, K(\boldsymbol{r}''t'', \boldsymbol{r}'t') \,, \quad (t > t'' > t') \,. \tag{361}$$

Another property of K is important — its dimension. Let $[Q]$ be the dimension of the quantity Q. A one-dimensional delta function $\delta(x)$ has dimension $[1/x]$, so the right side of (359) has dimension $L^{-d}T^{-1}\hbar$, where d is the dimension of $\mathfrak{C}$; the dimension of the left side is (energy)$\cdot[K]$, and therefore

$$[K] = L^{-d} \,. \tag{362}$$

(b) Green's Functions

When the Hamiltonian is time-independent, $U = e^{-iH(t-t')/\hbar}$, and the propagator then depends only on the interval $t-t'$. The preceding equations then simplify considerably. The propagator is now written as

$$K(\boldsymbol{r}, \boldsymbol{r}'; t) = \langle \boldsymbol{r}|e^{-iHt/\hbar}|\boldsymbol{r}'\rangle \; \theta(t) \,. \tag{363}$$

Let $\{\psi_{n\nu}(\boldsymbol{r})\}$ be a complete set of eigenfunctions of H, with energy eigenvalues E_n, and ν the additional quantum numbers beyond energy in the case of degeneracy:

$$\sum_{n\nu} \psi_{n\nu}(\boldsymbol{r})\psi^*_{n\nu}(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}') \,. \tag{364}$$

Then

$$K(\boldsymbol{r},\boldsymbol{r}';t)=\theta(t)\sum_{n,\nu}e^{-iE_nt/\hbar}\psi_{n\nu}(\boldsymbol{r})\psi^*_{n\nu}(\boldsymbol{r}')\ . \tag{365}$$

Equation (365) says that the propagator for a time-independent Hamiltonian is a Fourier series in time with the frequency spectrum $\{E_n/\hbar\}$. For this and other reasons, the Fourier transform of the propagator often plays an important role. To construct this transform, consider, first, the function defined by

$$f(E)=\int_C dz\frac{e^{-izt/\hbar}}{z-E}\ , \tag{366}$$

where E is real, $z=\xi+i\eta$, and the contour C traverses $-\infty<\xi<\infty$ just above the real axis. The integrand has a simple pole on the real axis at $z=E$, and is evaluated with Cauchy's theorem by closing the contour in the half-plane in which the exponential vanishes as $z\to\infty$. Let

$$e(z)=e^{-izt/\hbar}=e^{-i\xi t/\hbar}e^{\eta t/\hbar}\ . \tag{367}$$

If $t<0$, $e(z)\to 0$ in the upper half-plane, and after being closed the contour contains no singularities so the integral vanishes. But if $t>0$, $e(z)\to 0$ in the lower half-plane, in which case the closed contour includes the pole at $z=E$ and the integral equals $-2\pi ie^{-iEt/\hbar}$. In short,

$$f(E)=-2\pi ie^{-iEt/\hbar}\theta(t)\ . \tag{368}$$

When applied to (365),

$$K(\boldsymbol{r},\boldsymbol{r}';t)=\frac{i}{2\pi}\int_C dz\,e^{-izt/\hbar}\sum_{n,\nu}\frac{\psi_{n\nu}(\boldsymbol{r})\psi^*_{n\nu}(\boldsymbol{r}')}{z-E_n}\ . \tag{369}$$

Green's function for the time-independent Schrödinger equation is now defined as the integrand of this Fourier integral when $z=E+i\epsilon$:

$$G(\boldsymbol{r},\boldsymbol{r}';E)=\sum_{n,\nu}\frac{\psi_{n\nu}(\boldsymbol{r})\psi^*_{n\nu}(\boldsymbol{r}')}{E-E_n+i\epsilon}\ , \tag{370}$$

where ϵ is a *positive* infinitesimal. G has this name because it satisfies the inhomogeneous Schrödinger equation with a unit source term,

$$(E-H)G(\boldsymbol{r},\boldsymbol{r}';E)=\delta(\boldsymbol{r}-\boldsymbol{r}')\ , \tag{371}$$

which follows by applying $(E-H)$ to (370). According to (370), when E is extended to the complex plane, *Green's function has simple poles at the eigenvalues of the Hamiltonian,*[1] *with residues R_n whose spatial dependence give the corresponding eigenfunctions*:

$$R_n=\sum_\nu\psi_{n\nu}(\boldsymbol{r})\psi^*_{n\nu}(\boldsymbol{r}')\ . \tag{372}$$

[1]If the Hamiltonian has a spectrum that is partially or wholly continuous, then the poles coalesce into branch cuts. This will be elucidated in §4.4 and 8.2.

The inverse to (369) gives Green's function in terms of the propagator:

$$G(\boldsymbol{r},\boldsymbol{r}';E)=\frac{1}{i\hbar}\int_0^\infty dt\, e^{izt/\hbar}\,K(\boldsymbol{r},\boldsymbol{r};t)\;,\qquad z=E+i\epsilon\,. \tag{373}$$

The integral runs only over positive times because, by definition, this propagator K vanishes for $t<0$, and for that reason is called "causal" or "retarded." Propagators with other boundary conditions in time can also be defined.

The expressions (365) and (370) tell us that once the propagator, or equivalently, Green's function, is known, the energy spectrum and stationary state wave functions are also known, at least implicitly. In that sense, the propagator (or Green's function) provides a complete solution to the quantum mechanics of a system governed by a time-independent Hamiltonian. It should, therefore, come as no surprise that exact analytic expressions for these quantities are only known for a very small number of systems. On the other hand, because the propagator and Green's function are so rich in content, approximate expressions for them are often of much greater use than approximations to individual states.

(c) The Free Particle Propagator and Green's Function

The propagator and Green's function for free particles are important in their own right, and their evaluation is instructive.

The Hamiltonian of a free particle system is a sum of commuting terms, so the unitary operator U is a product of terms not only for each particle but also for each component of momentum. Hence it suffices to evaluate K for one particle moving in one dimension:

$$K(x,x';t)=\langle x|\exp(-i\hat{p}^2t/2m\hbar)|x'\rangle\;, \tag{374}$$

where $\hat{p}$ is the momentum operator. The description of a free particle must be translation invariant, so K can only depend on $x-x'$, and x' can be set to zero. Introducing the complete set of momentum eigenfunction of (176) gives

$$K(x;t)=\theta(t)\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\exp[i(px-p^2t/2m)/\hbar]\;. \tag{375}$$

As always, it pays to use dimensionless variables. Specific values of t and p define the classical characteristic distance $l=pt/m$, but in view of the de Broglie relation $p=\hbar/l$, this translates into a relation between length and time alone:

$$l=\sqrt{\hbar t/m}\;. \tag{376}$$

This prompts the introduction of the dimensionless length and momentum variables $\xi=x/l$ and $\eta=lp/\hbar$, in terms of which (375) is

$$K(x;t)=\theta(t)\,\frac{1}{2\pi l}\int_{-\infty}^{\infty}d\eta\,e^{i(\xi\eta-\frac{1}{2}\eta^2)}=\theta(t)\,\frac{1}{2\pi l}\,e^{i\xi^2/2}\int_{-\infty}^{\infty}d\eta\,e^{-i\eta^2/2}\;, \tag{377}$$

where a shift in η gave the last result. The dependence on x and t is now explicit, and the dimension is as expected from (362).

Integrals of the type appearing in (377) are called Gaussian integrals. Define

$$I(a)=\int_{-\infty}^{\infty}dx\,e^{-ax^2/2}=\sqrt{\frac{2\pi}{a}} \tag{378}$$

for a real and positive. For complex $a = |a|e^{i\theta}$, the integral is defined by analytic continuation provided $-\frac{1}{2}\pi \le \theta \le \frac{1}{2}\pi$:

$$I(a) = \sqrt{2\pi/|a|}\; e^{-i\theta/2} \; . \tag{379}$$

In (377), a is pure imaginary; integrals of this type are called Fresnel integrals, but we will use the name Gaussian for all integrals of this type. When $a = \pm i\lambda$, $\theta = \pm\frac{1}{2}\pi$,

$$\int_{-\infty}^{\infty} dx\, e^{\mp i\lambda x^2/2} = \sqrt{\frac{2\pi}{|\lambda|}} \begin{cases} 1/\sqrt{i} \\ \sqrt{i} \end{cases} \; . \tag{380}$$

This dependence on the sign of Im a must not be forgotten when the phase of the quantity being calculated matters.

The final result for the free particle propagator in one dimension is therefore

$$K(x;t) = \theta(t)\, \sqrt{\frac{m}{2\pi i\hbar t}}\; e^{ix^2 m/2\hbar t} \; . \tag{381}$$

As already stated, for N particles of various masses in three dimensions, the propagator is just a product of such factors:

$$K(\boldsymbol{r};t) = \theta(t)\; (2\pi i\hbar t)^{-3N/2} \prod_{n=1}^{N} (m_n)^{3/2}\; \exp\left(i\frac{r_n^2 m_n}{2\hbar t} \right) \; . \tag{382}$$

The form of the free particle Green's function does not have such a trivial dependence on the dimension d of the configuration space $\mathfrak{C}$. The reason is that Green's function is a wave emanating from a point source with the symmetry of the Laplacian in a Euclidean space of dimension d: it is a cylindrical wave when $d = 2$, a spherical wave when $d = 3$, etc.[1]

Consider the important case of a single particle in three dimensions. It turns out to be most convenient to not use the general definition (371), but rather Green's function for the Helmholtz equation,

$$(\nabla^2 + k^2) G_0(\boldsymbol{r} - \boldsymbol{r}'; k) = \delta(\boldsymbol{r} - \boldsymbol{r}') \; . \tag{383}$$

Here translation invariance is exploited, and the energy is written as $\hbar^2 k^2/2m$. Define the Fourier representation of G_0 as

$$G_0(\boldsymbol{r}; k) = \int \frac{d^3 q}{(2\pi)^3}\; g_k(\boldsymbol{q})\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \; . \tag{384}$$

Then (383) requires

$$(k^2 - q^2) g_k(\boldsymbol{q}) = 1 \; . \tag{385}$$

Without thought one might put $g = (k^2 - q^2)^{-1}$, but what then happens at $k^2 = q^2$? The answer is provided by (370): the singularity is to be averted by $k^2 \to k^2 + i\epsilon$, where ϵ is a *positive* infinitesimal. Hence

$$G_0(\boldsymbol{r}; k) = \int \frac{d^3 q}{(2\pi)^3}\; \frac{e^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{k^2 - q^2 + i\epsilon} \; . \tag{386}$$

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[1] Green's functions for the Helmholtz equation in an arbitrary number of dimensions are derived in A. Sommerfeld, *Partial Differential Equations in Physics,* Academic Press (1964), pp. 232–234.

Integrating over the orientation of $\boldsymbol{q}$, and *defining* k as positive, gives

$$\begin{aligned} G_0(\boldsymbol{r};k) &= \frac{1}{2\pi^2}\int_0^\infty q^2 dq\ \frac{\sin qr}{qr}\ \frac{1}{k^2-q^2+i\epsilon} \\ &= \frac{1}{8\pi^2 ri}\int_{-\infty}^{\infty} q\,dq\ \frac{e^{iqr}-e^{-iqr}}{(k+i\epsilon-q)(k+i\epsilon+q)}\ , \end{aligned} \tag{387}$$

where $r = |\boldsymbol{r}| \geq 0$. Now extend q to the complex plane; then $e^{\pm iqr} \to 0$ in the upper/lower half-planes of q, and the integral can, for the separate terms, be closed in these half-planes. The poles at $q = k \pm i\epsilon$ then give the final result

$$G_0(r;k) = -\frac{1}{4\pi}\ \frac{e^{ikr}}{r}\ , \qquad (d=3)\ . \tag{388}$$

As expected, this is a spherically symmetric wave centered at the origin. That the result could only depend on $|\boldsymbol{r}|$ was, of course, evident at the outset because the Laplacian is spherically symmetric. For the same reason g_k depends only on $|\boldsymbol{q}|$.

The fact that $G_0(r;k)$ is an *outgoing* wave merits some discussion. If the evaluation of (387) is repeated with $\epsilon \to -\epsilon$, the result is

$$G_0^{\rm adv}(r;k) = -\frac{1}{4\pi}\ \frac{e^{-ikr}}{r}\ , \tag{389}$$

which is a spherical wave *converging* onto the origin. This change in the sign of ϵ, when traced back to (366), there amounts to $z \to \xi - i\epsilon$, and in (368) to $\theta(t) \to \theta(-t)$! In short, the incoming wave Green's function (389) is related to propagation into the past, not the future, and for that reason this is called the *advanced* Green's function.

Green's function for a free particle in one dimension will also be useful:

$$G_0(x,x';k) = \frac{1}{2ki}\left[\theta(x-x')e^{ik(x-x')} + \theta(x'-x)e^{ik(x'-x)}\right] \tag{390}$$

$$= \frac{1}{2ik}e^{ik|x-x'|}\ , \qquad (d=1)\ . \tag{391}$$

The derivation is left as an exercise.

(d) Perturbation Theory

One of the most important applications of propagators is to the development of *perturbation theory.* Consider the situation in which the Hamiltonian H has the form $H_0 + V$, with the problem defined by H_0 being solvable, and V is in some sense small. Then it is natural to seek expressions for various quantities that depend on the "perturbation" V in terms of what is already known about H_0 by expanding in powers of V. What conditions H_0 and V must satisfy for such an expansion to be valid is often, indeed almost always, a sophisticated question, but for now assume that ignorance is bliss.

For the purpose of treating V as a perturbation, write[1] (359) as

$$[i\hbar\partial_{t_1} - H_0]K(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) = V(\boldsymbol{r}_1 t_1)K(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) + i\hbar\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta(t_1 - t_2)\ . \tag{392}$$

[1] If V is not diagonal in the coordinate representation, there is an obvious generalization requiring a further integration on the right-hand side.

Let K_0 be the propagator for the unperturbed problem:

$$[i\hbar\partial_{t_1} - H_0]K_0(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) = i\hbar\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta(t_1 - t_2) \; . \tag{393}$$

Then Eq. 392 implies

$$K(\boldsymbol{r}_1 t, \boldsymbol{r}_2 t_2) = K_0(\boldsymbol{r}_1 t_1, \boldsymbol{r}_2 t_2) + \frac{1}{i\hbar}\int d\boldsymbol{r}_3 dt_3 \, K_0(\boldsymbol{r}_1 t_1, \boldsymbol{r}_3 t_3) V(\boldsymbol{r}_3 t_3) K(\boldsymbol{r}_3 t_3, \boldsymbol{r}_2 t_2) \; , \tag{394}$$

or in an obvious and convenient shorthand,

$$K(1,2) = K_0(1,2) + \frac{1}{i\hbar}\int d3 \; K_0(1,3)V(3)K(3,2) \; . \tag{395}$$

To confirm this, apply $(i\hbar\partial_{t_1} - H_0)$ to (394) and use (393).

Equation (395) can be iterated by substituting the full expression for K into the integral:

$$\begin{aligned} K(1,2) = K_0(1,2) &+ \frac{1}{i\hbar}\int d3 \; K_0(1,3)V(3)K_0(3,2) \\ &+ \frac{1}{(i\hbar)^2}\int d3\, d4 \; K_0(1,3)V(3)K_0(3;4)V(4)K(4,2) \; . \end{aligned} \tag{396}$$

This is still exact. The iteration can be repeated until the desired power of V is reached. The expansion in powers of V is thus

$$\begin{aligned} K(1,2) = K_0(1,2) &+ \frac{1}{i\hbar}\int d3 \; K_0(1,3)V(3)K_0(3,2) \\ &+ \frac{1}{(i\hbar)^2}\int d3\, d4 \; K_0(1,3)V(3)K_0(3,4)V(4)K_0(4,2)\ldots \; , \end{aligned} \tag{397}$$

or in a still more compact notation:

$$K = K_0\left(1 + \sum_{n=1}^{\infty}(i\hbar)^{-n}(VK_0)^n\right) \; . \tag{398}$$

This series is basic to time-dependent perturbation theory, and is used in a broad range of phenomena in many branches of physics. Here and as in quantum field theory, it leads to the famous Feynman diagrams, which are graphical mnemonics that greatly simplify the evaluation of the terms in the series.

A very important perturbation expansion in powers of V also exists for Green's function. This expansion will now be developed without paying heed to whether it is legitimate, for that is a complicated issue which will be taken up in the context of specific problems. One point can be made right now, however. Replace V by λV, where λ is a parameter that can be set to 1 in the end. The naive perturbation expansions assume that the quantities of interest, such as Green's function, the energy, the wave function, etc., are analytic functions of the complex variable λ inside the unit circle. Often a simple physical argument demonstrates that this condition is not met, and sometimes a sophisticated consideration will lead to such a conclusion. But in a host of important problems it is simply not known whether a power series expansion is valid, and it is still used because it seems to work, or nothing more sophisticated is practical.

The derivation of the perturbation series is facilitated by introducing an operator $\mathcal{G}$ called *the resolvent*. It is motivated by Eq. 370:

$$\mathcal{G}(z) \;=\; \sum_{n\nu} |n\nu\rangle \, \frac{1}{z - E_n} \, \langle n\nu| \;=\; \sum_{n} \frac{P_n}{z - E_n} \;\equiv\; \frac{1}{z - H} \; . \tag{399}$$

Here P_n is the projection operator onto *all* states of energy E_n, and the last expression is a very convenient form, as we shall soon see. The resolvent is well-defined as long as z is not on the real axis because the spectrum of the Hermitian operator H is real. As is clear from (370), Green's function is just the set of all matrix elements of the resolvent in the coordinate representation when $z = E + i\epsilon$:

$$G(\boldsymbol{r}, \boldsymbol{r}'; E) = \langle \boldsymbol{r} | \mathcal{G}(E + i\epsilon) | \boldsymbol{r}' \rangle \; . \tag{400}$$

In terms of $\mathcal{G}$, the inhomogeneous Schrödinger equation (371) is simply

$$(z - H)\mathcal{G}(z) = 1 \; . \tag{401}$$

The perturbation expansion follows from an identity whose derivation is left as an exercise. For any two operators A and B,

$$\frac{1}{A - B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A - B} = \frac{1}{A} + \frac{1}{A - B} B \frac{1}{A} \; . \tag{402}$$

These expressions only make sense, of course, if the denominators have no vanishing matrix elements; as before, this is accomplished by generalizing the energy to a complex variable. Now define $\mathcal{G}_0$, the "unperturbed" counterpart of $\mathcal{G}$, by

$$\mathcal{G}_0(z) = \frac{1}{z - H_0} \; . \tag{403}$$

The matrix elements of this resolvent form Green's function for the Schrödinger equation belonging to the unperturbed Hamiltonian H_0. Setting $A = z - H_0$ and $B = V$ in (402) thus gives

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G} \; , \tag{404}$$

which is shorthand for the integral equation

$$G(\boldsymbol{r}, \boldsymbol{r}') = G_0(\boldsymbol{r}, \boldsymbol{r}') + \int d\boldsymbol{s} \, G_0(\boldsymbol{r}, \boldsymbol{s}) V(\boldsymbol{s}) G(\boldsymbol{s}, \boldsymbol{r}') \; , \tag{405}$$

where E has been suppressed, and all the coordinates range over the whole of configuration space. The expansion of the exact resolvent in powers of the perturbation V again ensues by iteration:

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V (\mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}) \; , \tag{406}$$

which is exact. Repeated iteration, and the assumption that terms beyond some given order are negligible, then yields the perturbation series:

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}_0 V \mathcal{G}_0 + \ldots \; . \tag{407}$$

The expansion of Green's function in powers of the perturbation is often called the *Born series.* Only the first term in the expansion was used by Born in the paper that gave both the first treatment of a scattering problem in quantum mechanics, and (in a footnote) the *Born interpretation* of the wave function as a probability amplitude.

2.7 The Path Integral

The path integral is widely used in quantum field theory and statistical mechanics, and has also proven to be a powerful tool in numerical computations. On the other hand, in the simpler problems with which we deal in this volume, it must be said that the path integral is rarely a more powerful computational tool than those that emerge from the older formulations of quantum mechanics, or even competitive with them. (It should also be said that when ambiguities arise in the path integral formulation, and they do, these are ultimately resolved by comparing with canonical quantization or the Schrödinger equation.) Nevertheless, because of the powerful concepts on which it is based, and the widespread use just mentioned, acquaintance with the path integral is indispensable.

(a) The Feynman Path Integral

For systems composed of particles (as compared to dynamical fields), Feynman's path integral expresses the propagator as a coherent sum of an infinite number of amplitudes over *all* paths in configuration space, and not just those dictated by the classical equations of motion. As the classical limit is approached, the paths in the immediate neighborhood of a true classical path become ever more dominant. The path integral thus yield important insights into the connection between classical and quantum mechanics, quite apart from its other virtues. This connection will be developed in detail in §2.8.

This formulation of quantum mechanics has the remarkable feature of not using operators in Hilbert space. Rather, it constructs probability amplitudes *ab initio* from the classical concept of paths in configuration space, albeit paths that are not constrained by classical mechanics. As we will be deriving the path integral from the older versions of quantum mechanics, we will start from the Hilbert space formulation.

Consider, first, the simplest situation, a single particle in one dimension, with the Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}, t) \equiv T(\hat{p}) + V(\hat{x}) \ , \tag{408}$$

where the notation $\hat{p}$, etc., emphasizes that these objects are operators. The generalization to interacting particles in three dimensions is straightforward, though velocity-dependent interactions, such as those with electromagnetic fields, involve some complications.

The object of interest is the propagator,

$$K(b,a) = \langle x_b | U(t_b, t_a) | x_a \rangle \, \theta(t_b - t_a) \ ; \qquad a \equiv (x_a t_a) \ , \ b \equiv (x_b t_b) \ . \tag{409}$$

The path integral representation for K is obtained by:

1. breaking the evolution from a to b into a large sequence of κ small forward steps in time of duration τ by means of the composition law (238) for U;

2. evaluating each small step explicitly;

3. showing that these steps sum to the form $\sum_P \exp(iS/\hbar)$, where S is the classical action for some path P composed of linear segments from a to b;

4. taking the limit, to be called Lim, defined by

$$\mathsf{Lim} : \tau \to 0, \quad \kappa \to \infty, \quad \kappa\tau = t_b - t_a \ , \tag{410}$$

with $t_b - t_a$ held fixed.

The sequence of steps is a product of κ unitary transformations:

$$K(b,a) = \langle x_b | U(t_b, t_b - \tau) \dots U(t_a + 2\tau, t_a + \tau) U(t_a + \tau, t_a) | x_a \rangle \ . \tag{411}$$

Define

$$t_a \equiv t_0, \ t_k = t_0 + k\tau, \ t_b \equiv t_\kappa; \qquad x_a \equiv x_0, \ x_b \equiv x_\kappa \ . \tag{412}$$

On introducing $\kappa - 1$ sets of intermediate states $\{|x_k\rangle\}$, (411) becomes

$$\begin{aligned} K(b,a) = \int_{-\infty}^{\infty} dx_{\kappa-1} \dots dx_2 dx_1 \ \langle x_\kappa | e^{-iH(t_{\kappa-1})\tau/\hbar} | x_{\kappa-1} \rangle \dots \\ \dots \langle x_2 | e^{-iH(t_1)\tau/\hbar} | x_1 \rangle \langle x_1 | e^{-iH(t_0)\tau/\hbar} | x_0 \rangle \ . \end{aligned} \tag{413}$$

With $\tau \to 0$ anticipated, the time argument of H in any step can be taken anywhere in the interval, and the lower end was chosen. Unless V has a discontinuous time dependence, this is legitimate, but not when V is velocity-dependent.

It is tempting to replace $e^{-iH\tau/\hbar}$ by $1 - iH\tau/\hbar$. This would, however, spoil the unitary property as expressed in the composition law (238), and thereby abandon the superposition principle. An approximation valid as $\tau \to 0$ is thus needed which maintains unitarity. In addition, as T and V are diagonal in the momentum and coordinate representations, respectively, this approximation should, ideally, replace $e^{-iH\tau/\hbar}$ by a product of unitary operators that are diagonal in these incompatible representations. This wish list is met by the Baker-Campbell-Hausdorff (BCH) theorem[1]

$$e^A e^B = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{12}\left([A,[A,B]] - [B,[A,B]]\right) \dots \right) \ , \tag{414}$$

where A and B are operators in Hilbert space, and $\dots$ alludes to multiple commutators of ever higher order. In our case, both A and B are proportional to τ, so the terms beyond $A + B$ are of order τ^2 or smaller, and permit the approximation

$$e^{-iH\tau/\hbar} \simeq e^{-iT\tau/\hbar} \, e^{-iV\tau/\hbar} \ . \tag{415}$$

Hence

$$\begin{aligned} \langle x_{k+1} | e^{-iH(t_k)\tau/\hbar} | x_k \rangle &= \langle x_{k+1} | e^{-iT\tau/\hbar} | x_k \rangle \, e^{-iV(x_k t_k)\tau/\hbar} \\ &= \sqrt{\frac{m}{2\pi i\hbar\tau}} \exp\left[\frac{i}{\hbar} \left(\frac{(x_{k+1} - x_k)^2 m}{2\tau} - \tau V(x_k t_k) \right) \right] \ , \end{aligned} \tag{416}$$

[1]The simplest special case is when $[A,B]$ commutes with both A and B, so that all terms beyond $[A,B]$ vanish. It has many applications, and the proof is the subject of Prob. 13.

where the free particle propagator (381) was used in the second step. Returning to (413) gives

$$K(b,a) = \mathsf{Lim}\left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{1}{2}\kappa} \int_{-\infty}^{\infty} dx_{\kappa-1}\ldots dx_1 \times \exp\left[\frac{i\tau}{\hbar}\sum_{k=0}^{\kappa-1}\left(\frac{(x_{k+1}-x_k)^2 m}{2\tau^2} - V(x_k t_k)\right)\right] . \quad (417)$$

Imagine now a path $x(t)$ composed of linear segments from a to b passing through $(x_1,\ldots,x_{\kappa-1})$ at $(t_1,\ldots,t_{\kappa-1})$, as in the *integrand* of (417), and depicted in Fig. 2.4. The ratio $(x_{k+1}-x_k)/\tau$, as $\tau\to 0$, is the velocity $\dot{x}(t_k)$ in this step. Therefore

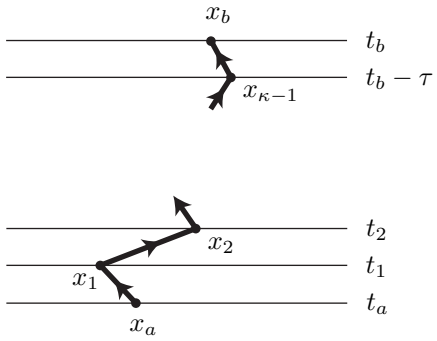

FIG. 2.4. Coordinates involved in the path integral (Eq. 417).

$$\lim_{\tau\to 0}\left(\frac{(x_{k+1}-x_k)^2 m}{2\tau^2} - V(x_k t_k)\right) = \frac{1}{2}m[\dot{x}(t_k)]^2 - V(x(t_k)t_k) = L(x(t_k),\dot{x}(t_k),t_k) , \quad (418)$$

i.e., *the Lagrangian* of the system at (x_k,t_k). The sum on k in (417) is therefore a discrete approximation to the time integral of the Lagrangian from a to b over the particular path $x(t)\equiv(x_a t_a;\ldots;x_k t_k;\ldots;x_b t_b)$,

$$\mathsf{Lim}\sum_{k=0}^{\kappa-1} L(t_0+k\tau) = \int_{t_a}^{t_b} dt' L(x(t'),\dot{x}(t'),t') \equiv S_{ba}[x(t)] , \quad (419)$$

where $F[x(t)]$ denotes a functional of $x(t)$. *The functional $S_{ba}[x(t)]$ is the classical action for motion along the arbitrary path $x(t)$.* Hence (417) is

$$K(b,a) = \mathsf{Lim}\left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{1}{2}\kappa}\int_{-\infty}^{\infty} dx_{\kappa-1}\ldots\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx_1\ \exp\left(\frac{i}{\hbar}S_{ba}[x(t)]\right) . \quad (420)$$

In this expression the path $x(t)$ is unrestricted except at the and points, and is not just one selected by the classical equation of motion, i.e., not just a path that minimizes the action. In the limit $\tau\to 0$, the integrals over the intermediate points $(x_1,\ldots,x_{\kappa-1})$ therefore include all paths from a to b. The last two sentences,

and Eq. 420, *define* what is meant by the path integral. Following Feynman, it is customary to write this last equation as

$$K(b,a) = \int_a^b \mathcal{D}(x(t))\ \exp\left(\frac{i}{\hbar}S_{ba}[x(t)]\right)\ , \tag{421}$$

where the meaning of the differential, or measure, $\mathcal{D}(x(t))$, and the integration symbol, are to be understood by referring back to (420).

The argument just given pays even less heed to mathematical discipline than is customary in theoretical physics, for it is reasonable to fear that here there could be fatal booby-traps because the set of all paths surely contains exotica that will not submit to routine integration. One is banking on the hope that that such paths will produce sufficiently rapid oscillations in $e^{iS/\hbar}$ to not contribute in the limit. This is not unreasonable, because the phase in (417) oscillates rapidly if the path is sufficiently erratic to violate

$$|x_{k+1} - x_k| \lesssim \sqrt{\hbar\tau/m}\ . \tag{422}$$

For a fixed time-slice parameter τ, a sufficiently large mass will suppress paths that are far from the differentiable classical path. (Indeed, the formal classical limit $\hbar \to 0$ forces the path to be smooth, a fact that will be explored in more detail in the following section.) And for any mass, there is a τ sufficiently small to suppress paths that jump about in space by an amount that violates (422). This argument does not pretend to be mathematically satisfactory; readers seeking such a treatment should consult the literature cited at the end of this chapter.

The generalization to more particles in three dimensions in the absence of velocity-dependent forces is straightforward; $x(t)$ is simply replaced by a path in the configuration space of the system. The evaluation of such path integrals is anything but straightforward, of course.

When there are velocity-dependent forces, the discretization of the evolution $a \to b$ involves a subtle point. This is illustrated by the important example of a particle of charge e in the presence of a magnetic field with vector potential $\boldsymbol{A}(\boldsymbol{r})$. (Time-dependent magnetic and electric fields do not produce any further problems.) The classical Lagrangian for this system is

$$L = \frac{1}{2}m[\dot{\boldsymbol{r}}(t)]^2 - V(\boldsymbol{r}) + \frac{e}{c}\dot{\boldsymbol{r}}\cdot\boldsymbol{A}(\boldsymbol{r})\ . \tag{423}$$

The propagator $K(b,a)$ must satisfy a condition imposed by gauge invariance. Because of the definition (354) and (355) of the propagator, and the gauge transformation (349) of wave function, this condition is

$$K(\boldsymbol{r}t,\boldsymbol{r}'t') \to e^{ie\chi(\boldsymbol{r})/\hbar c}K(\boldsymbol{r}t,\boldsymbol{r}'t')\,e^{-ie\chi(\boldsymbol{r}')/\hbar c}\ . \tag{424}$$

The generalization of (420) when the Lagrangian is (423) must conform with this. It turns out that in slicing the time evolution the vector potential must be evaluated at the midpoint between $\boldsymbol{r}_k$ and $\boldsymbol{r}_{k+1}$ to meet this requirement.

(b) The Free-Particle Path Integral

Although we already know the propagator for free particles (recall Eq. 381), it is instructive to go through the much more demanding task of finding it by means of

the path integral. For that matter, two separate derivations will be given, the first of which actually avoids doing the path integral.

As we already learned, when there are no interactions nothing is gained by treating more than one particle in more than one dimension. Let $x(t)$ be an arbitrary path, $Q(t)$ the classical path from (x_a, t_a) to (x_b, t_b), and

$$y(t) = x(t) - Q(t) \tag{425}$$

be the deviation from the classical path. In the variable y, all paths start and end at $y = 0$ because all paths $x(t)$ start at a and end at b.

First-order deviations from the classical path leave the action unchanged, and therefore the action for the arbitrary path $x(t)$ is

$$S[Q(t) + y(t)] = \tfrac{1}{2}m \int_{t_a}^{t_b} dt\, [\dot{Q}^2(t) + \dot{y}^2(t)] \,. \tag{426}$$

The first term is the classical action,

$$S_{\rm cl}(b,a) = \int_{t_a}^{t_b} dt\, \tfrac{1}{2}m\dot{Q}^2(t) = \frac{m}{2}\,\frac{(x_b - x_a)^2}{t_b - t_a} \,. \tag{427}$$

This action could also be expressed as $\frac{1}{2}p(x_b - x_a)$, but this would not make sense in this quantum mechanical context because the momentum and position cannot be specified simultaneously. The action must be expressed in terms of the initial and final coordinates and the elapsed time, as required by the definition of the propagator.

The separation of arbitrary paths into the classical path and the departure therefrom thus results in

$$K(b,a) = F(t_b - t_a)\, \exp\left(\frac{i}{\hbar} S_{\rm cl}(b,a)\right) \,, \tag{428}$$

where $F(t_b - t_a)$ is the integral over all paths from $y = 0$ back to $y = 0$ during the interval $t_b - t_a$:

$$F(t_b - t_a) = \int_{t_a, y=0}^{t_b, y=0} \mathcal{D}(y(t)) \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \tfrac{1}{2}m\dot{y}^2(t)\right) \,. \tag{429}$$

Evaluation of the path integral can in this case (and some others) be evaded by a trick due to Feynman. It exploits the composition law (361), the fact that F is the propagator from the origin to the origin, and (428):

$$\begin{aligned} F(t) &= \int_{-\infty}^{\infty} dy\; K(0,t;y,t')K(y,t';0,0) && (430)\\ &= F(t-t')F(t') \int_{-\infty}^{\infty} dy\; \exp\left[iy^2\left(\frac{1}{t-t'} + \frac{1}{t'}\right)\frac{m}{2\hbar}\right] \\ &= F(t-t')F(t')\, (2\pi i\hbar/m)^{\frac{1}{2}} \sqrt{t'(t-t')/t} \,. && (431) \end{aligned}$$

Therefore

$$F(t_b - t_a) = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}} \,. \tag{432}$$

When combined with (428) the known result, Eq. 381, is recovered:

$$K(b,a) = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}\, \exp\left(\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)}\right) \ . \tag{433}$$

A brute-force evaluation of the free-particle path integral is more instructive, however, because it hints at what must be done in more difficult problems, or when the path integral is computed numerically in problems where no analytic approach is known or practical.

From the definition (417) et seq. of the path integral, (429) is

$$F(t_b - t_a) = \mathsf{Lim}\left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{1}{2}\kappa} \int_{-\infty}^{\infty} dy_{\kappa-1}\ldots dy_1 \times \exp\left(\frac{im}{2\hbar\tau}\sum_{k=0}^{\kappa-1}(y_{k+1} - y_k)^2\right) . \tag{434}$$

Introduce dimensionless variables, i.e.,

$$\eta_\kappa = y_k\sqrt{m/\hbar\tau}\ , \tag{435}$$

so that

$$F(t_b - t_a) = \mathsf{Lim}\left(\frac{m}{\hbar\tau}\right)^{\frac{1}{2}} \left(\frac{1}{2\pi i}\right)^{\frac{1}{2}\kappa} \int_{-\infty}^{\infty} d\eta_{\kappa-1}\ldots d\eta_1 \times \exp\left(\frac{i}{2}\sum_{k=0}^{\kappa-1}(\eta_{k+1} - \eta_k)^2\right) . \tag{436}$$

The integral is now a pure number — the complete dependence on $\hbar$ and m is in the factor $\sqrt{m/\hbar}$, a fact that will be important when we examine the classical limit in the next section.

The argument of the exponential in (436) is a quadratic form, which, after it is diagonalized, reduces F to a product of Gaussian integrals. In detail,

$$\sum_{k=0}^{\kappa-1}(\eta_{k+1} - \eta_k)^2 = 2(\eta_1^2 + \eta_2^2 + \ldots + \eta_{\kappa-1}^2 - \eta_1\eta_2 - \eta_2\eta_3 - \ldots \eta_{\kappa-2}\eta_{\kappa-1}) \tag{437}$$

because $y_0 = y_\kappa = 0$. Next, define the symmetric matrix

$$\Lambda = \begin{pmatrix} 2 & -1 & 0 & \ldots & & \\ -1 & 2 & -1 & & & \\ 0 & -1 & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & -1 \\ & & & & -1 & 2 \end{pmatrix} , \tag{438}$$

in terms of which

$$\sum_{k=0}^{\kappa-1}(\eta_{k+1} - \eta_k)^2 = \sum_k \zeta_k^2\lambda_k\ , \tag{439}$$

where $\{\zeta_k\}$ and $\{\lambda_k\}$ are the eigenvectors and eigenvalues of Λ. The new element of integration is $d\zeta_1 \dots d\zeta_{\kappa-1}$ because the transformation from $\{\eta_k\}$ to $\{\zeta_k\}$ is orthogonal. All λ_k are positive, and therefore (380) gives

$$F(t) = \mathsf{Lim}\, \sqrt{\frac{m}{2\pi i\hbar\tau}} \prod_{k=1}^{\kappa-1} \int_{-\infty}^{\infty} \frac{d\zeta_k}{\sqrt{2\pi i}}\, e^{\frac{1}{2} i\zeta_k^2 \lambda_k} \tag{440}$$

$$= \mathsf{Lim}\, \sqrt{\frac{m}{2\pi i\hbar\tau\ \det\Lambda}}\ , \tag{441}$$

where

$$\det\Lambda = \prod_k \lambda_k \tag{442}$$

is the determinant of Λ. By computing $\det\Lambda$ for small values of κ, one quickly concludes that[1]

$$\det\Lambda = \kappa + 1\,, \tag{443}$$

and Eq. 432 reappears when Lim is taken because $\kappa\tau = t_b - t_a$.

The heuristic argument made about the paths that dominate when there is a potential [recall Eq. 422, etc.] is manifestly correct in the free-particle case. From (440), and the fact that the eigenvalues λ_k are of order one, it follows that the spatial dispersion of the paths about the classical straight line is of order $|\zeta| \simeq 1$, or $|\delta y| \simeq \sqrt{\hbar\tau/m}$, in agreement with (422).

2.8 Semiclassical Quantum Mechanics

Quantum mechanics must somehow incorporate classical mechanics in the limit $\hbar \to 0$. Other examples of such relationships are common in physics. For example, Newton's equations of motion arise directly from their relativistic generalization by taking the limit $c \to \infty$ in the latter. The relation between classical and quantum mechanics is far less straightforward, however. At the formal level, the classical equations of motion do not arise out of Schrödinger's or Heisenberg's equations by simply setting $\hbar \to 0$. The mathematical reason is that that the probability amplitudes of quantum mechanics are highly singular as $\hbar \to 0$, as is evident in the form $\sum[\exp(iS/\hbar)]$ of the path integral, which reveals an essential singularity at $\hbar = 0$. From a conceptual viewpoint there is a much deeper chasm between classical and quantum mechanics than that between relativistic and nonrelativistic classical mechanics. The complexity of the mathematical connection between classical and quantum mechanics seems to reflect this profound conceptual separation.

The link to classical mechanics is more direct in the path integral than in the Hilbert space formulation, because the former is based on the classical concept of paths in configuration space. This link relies on the formulation of classical mechanics due to Hamilton and Jacobi, and for that reason we begin, in subsection (a), with a sketch of Hamilton-Jacobi theory.[2] As the derivation of the semiclassical

[1] For a proof of (443) that generalizes to more difficult cases, see Prob. 14.

[2] Indeed, Schrödinger's discovery of his wave equation stemmed from this connection; the Hamilton-Jacobi equation is the first equation in his first paper.

propagator involves some intricate analysis, we then present, in subsection (b), a heuristic semiclassical approximation to the Schrödinger wave function which is intuitively attractive but of limited validity. A description of the semiclassical propagator is then given in subsection (c), with detailed derivations postponed to subsection (d).

(a) Hamilton-Jacobi Theory

In classical mechanics, all possible motions of a system are determined by its *Lagrangian*, $L(q(t), \dot{q}(t), t)$. Here $q(t)$ is a shorthand for a point $(q_1(t), \ldots, q_f(t))$ in the configuration space $\mathfrak{C}_f$, and f the number of degrees of freedom. For an N-particle system, the relation to the notation of the earlier sections is $(q_1, q_2, q_3) = \boldsymbol{r}_1$, $m_{1,2,3} = m_1$, etc. In this section q_i and the conjugate momenta p_i are always c-numbers, never operators, whether classical or quantum mechanics is under discussion.

The *classical action* is the integral of L along a trajectory *allowed* by the equations of motion, from a configuration $q_a = (q_1(t_a), \ldots, q_f(t_a))$ at time t_a to another point q_b in $\mathfrak{C}_f$ at time t_b :

$$S(q_b t_b; q_a t_a) \equiv S(b, a) = \int_{t_a}^{t_b} dt\, L(q(t), \dot{q}(t), t) \; . \tag{444}$$

This is not to be confused with the action appearing in the path integral, which includes all paths, whether or not permitted classically.

The most familiar way of selecting a particular classical trajectory is to specify the initial q_i and p_i , but this does not translate into quantum mechanics because of the uncertainty principle. A classical formulation does exist which evades this problem, namely, that based on $S(b, a)$, for it selects a particular trajectory by specifying the initial and final configurations (q_a, t_a) and (q_b, t_b), which corresponds to the specification of a particular propagator $K(b, a)$.

As $S(b, a)$ is only a function of the initial and final coordinates, it remains to find the corresponding momenta. For that purpose, consider arbitrary variations δq:

$$\delta S(b, a) = \int_{t_a}^{t_b} dt \; \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) \delta q_i \;\; + \;\; \frac{\partial L}{\partial \dot{q}_i} \delta q_i \Big|_{t_a}^{t_b} \; . \tag{445}$$

The integral vanishes thanks to Lagrange's equations. Because $p_i = \partial L / \partial \dot{q}_i$, the end points contribute

$$\delta S(b, a) = p_{b,i}\, \delta q_i(t_b) - p_{a,i}\, \delta q_i(t_a) \, , \tag{446}$$

and therefore

$$p_{b,i} = \frac{\partial}{\partial q_{b,i}} S(b, a) = \; p_{b,i}(q_b t_b; q_a t_a) \; , \tag{447}$$

$$p_{a,i} = - \frac{\partial}{\partial q_{a,i}} S(b, a) = \; p_{a,i}(q_b t_b; q_a t_a) \; . \tag{448}$$

Note that these momenta are functions of the initial and final configurations.

The change of the action when the time at end point b varies is

$$\frac{dS}{dt_b} = L(t_b) = \frac{\partial S}{\partial t_b} + \frac{\partial S}{\partial q_{b,i}}\dot{q}_{b,i} = \frac{\partial S}{\partial t_b} + p_{b,i}\dot{q}_{b,i} \; ; \tag{449}$$

at b, the relation between the Hamiltonian and Lagrangian is

$$H(t_b) = p_{b,i}\, \dot{q}_{b,i} - L(t_b) \; . \tag{450}$$

Therefore

$$\frac{\partial S}{\partial t_b} + H(t_b) = 0 \; . \tag{451}$$

For now, we fix the initial configuration (q_a, t_a), and concentrate on the variation with the variables (q_b, t_b), called simply (q, t). The *Hamilton-Jacobi equation* is nothing but (451) after the momenta in $H(q, p, t)$ are eliminated by use of (447):

$$\frac{\partial S}{\partial t} + H\left(q_1, \ldots, q_f; \frac{\partial S}{\partial q_1}, \ldots, \frac{\partial S}{\partial q_f}; t\right) = 0 \; . \tag{452}$$

As an important example, consider a system of charged particles exposed to an electromagnetic field, and having mutual interactions that are not velocity-dependent. The Hamiltonian and Lagrangian are

$$H = \sum_i \frac{1}{2m_i}\left[p_i - \Phi_i(t)\right]^2 + V(q_i, \ldots, q_f; t) \; , \qquad \Phi_i(t) \equiv \frac{e_i}{c} A_i(t) \; , \tag{453}$$

$$L = \sum_i \left(\tfrac{1}{2} m_i\, \dot{q}_i^2 + \dot{q}_i \Phi_i(t)\right) - V \; , \tag{454}$$

where $A_i(t)$ is a component of the vector potential evaluated at the position particle i. The potential V describes the interactions between the particles, and any applied electric field. According to (452), for this system the Hamilton-Jacobi equation is

$$\frac{\partial S}{\partial t} + \sum_i \frac{1}{2m_i}\left(\frac{\partial S}{\partial q_i} - \Phi_i\right)^2 + V = 0 \; . \tag{455}$$

The velocities are found from $\dot{q}_i = \partial H / \partial p_i$ and (447):

$$\dot{q}_i = \frac{1}{m_i}\left(\frac{\partial S}{\partial q_i} - \Phi_i\right) \; . \tag{456}$$

The Hamilton-Jacobi equation thus offers a description of dynamics that is very different from those given by Hamilton's or Lagrange's equations of motion. The latters' multitudes of ordinary differential equations are replaced by just *one* partial differential equation. This equation is of first order in time, has $f + 1$ independent variables, $(q_1, \ldots, q_f)$ and t, and one dependent variable S. This does smell like Schrödinger's equation in configuration space: the same order in time, the same independent variables, and one dependent variable, the wave function ψ. Of course, there is one obvious and crucial difference: Schrödinger's equation is linear in ψ (the superposition principle!), whereas the Hamilton-Jacobi equation is nonlinear in S.

There is also a remarkable analogy between the solution $S(b,a)$ of the Hamilton-Jacobi equation and the propagator $K(b,a)$: both handle whole families of trajectories in one fell swoop. Given initial data at time t_0 as a continuous function $S(q,t_0)$ in $\mathfrak{C}_f$, the partial differential equation (452) will manufacture $S(q,t)$ in the future.

Hamilton gave an elegant geometrical depiction of how the trajectories of particles emerge from this continuum formulation of point mechanics by drawing an analogy to the way in which the rays of geometrical optics emerge from wave optics. For our purpose, it suffices to consider a time-independent Hamiltonian, equal masses and no vector potential. Then

$$S(q,t) = W(q) - Et \ , \tag{457}$$

where E is the energy, and (455) simplifies to

$$|\boldsymbol{\nabla} S| = |\boldsymbol{\nabla} W| = \sqrt{2m(E-V)} \ , \tag{458}$$

where $\boldsymbol{\nabla}$ is the gradient in f-dimensional Euclidean space, i.e., the configuration space $\mathfrak{C}_f$.

Consider, first, the family of surfaces $W(q) = \text{const.}$, which coincide with the surfaces of constant $S(q,t)$ at $t = 0$. As time increases, the surfaces of constant S move in obedience to (457). Take a particular surface $W(q) = W_0$; the surface of S that originally satisfied $S = W_0$ must move by time t to coincide with the surface $W(q) = W_0 + Et$. In short, to visualize the motion of S it suffices to visualize the family $\mathcal{F}$ of surfaces of constant $W(q)$ (see Fig. 2.5).

Furthermore, given one member $\mathcal{F}_0$ (say $W(q) = W_0$) of $\mathcal{F}$, all others can be constructed from it as follows. Eq. 458 specifies the gradient of W throughout $\mathfrak{C}_f$; erect a vector $\boldsymbol{u}$ normal to $\mathcal{F}_0$ of length ds at each point, where

$$ds = \frac{dW}{\sqrt{2m[E-V(q)]}} \ . \tag{459}$$

Then the locus of the end points of these vectors $\boldsymbol{u}$ is the surface on which $W(q) = W_0 + dW$. The continuation of this process constructs the whole family $\mathcal{F}$.

The motion of a surface of constant $S(q,t)$ is found from $dW = Edt$; such a surface therefore moves normal to itself in the direction given by the sign of E and with a velocity of magnitude

$$\frac{ds}{dt} = \frac{E}{\sqrt{2m[E-V(q)]}} \ . \tag{460}$$

If we think of the surfaces $S = \text{const.}$ as wave-fronts, then ds/dt is analogous to the phase velocity.

Finally, because

$$p_i = \partial W(q)/\partial q_i \ , \tag{461}$$

the family of curves normal to the family of surfaces $\mathcal{F}$ are the trajectories; i.e., the set of paths in $\mathfrak{C}_f$ along any one of which a system point $q(t)$ moves in accordance with the laws of mechanics. The magnitude of the velocity of any particular motion as it passes through q is not ds/dt, however, but $\sqrt{2(E-V)/m}$ according to (461) and (458). Therefore, in its motion along a trajectory, a moving point $q(t)$ does not stay on one surface $S = \text{const.}$

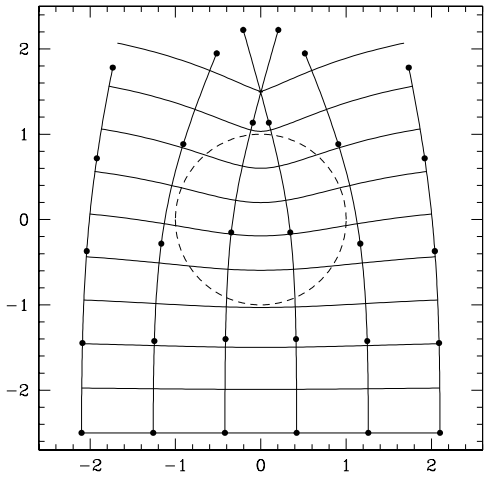

FIG. 2.5. Solution of the Hamilton-Jacobi equation in two dimensions for the potential $V(x,y) = -(1+x^2+y^2)^{-1}$, on the dashed circle $V = -\frac{1}{2}$. The dots are the positions of particles at $t = T, 2T, 3T, 4T$, which started at $t = 0$ with equal velocities in the y-direction at $y = -2.5$, and form trajectories that are everywhere normal to the surfaces of constant W, as shown. Note that these positions at any time after $t = 0$ do not stay on a single surface of constant W (see discussion following Eq. 460). The surfaces $W =$ const. develop cusps when trajectories cross, which is of importance in the construction of the semiclassical propagator (see Eq. 480 et seq.).

(b) The Semiclassical Wave Function

The earliest papers by de Broglie and Schrödinger made it evident that $\hbar$ appears explicitly in quantum mechanical amplitudes in the form $\exp(i\Theta/\hbar)$. This raises the question of whether there are circumstances under which Θ does not depend on $\hbar$, and if so, whether Θ then has a meaning in classical mechanics. This question is answered by the *Ansatz* due to Brillouin and Wentzel,

$$\psi(q,t) = e^{i\Theta(q,t)/\hbar} \,. \tag{462}$$

For the Hamiltonian (453), the Schrödinger equation is

$$\left(\sum_i \frac{1}{2m_i} \left(\frac{\hbar}{i} \frac{\partial}{\partial q_i} - \Phi_i \right)^2 + V(q) \right) \psi = i\hbar \frac{\partial \psi}{\partial t} \,. \tag{463}$$

A short calculation shows that

$$\left(\frac{\hbar}{i} \frac{\partial}{\partial q_i} - \Phi_i \right)^2 e^{i\Theta/\hbar} = \left[\left(\frac{\partial \Theta}{\partial q_i} - \Phi_i \right)^2 + \frac{\hbar}{i} \left(\frac{\partial^2 \Theta}{\partial q_i^2} - \frac{\partial \Phi_i}{\partial q_i} \right) \right] e^{i\Theta/\hbar} \,. \tag{464}$$

In the gauge $\boldsymbol{\nabla} \cdot \boldsymbol{A} = 0$, $\partial \Phi_i / \partial q_i = 0$. Having made no approximation, the Schrödinger equation thus requires Θ to satisfy

$$\frac{\partial \Theta}{\partial t} + \sum_i \frac{1}{2m_i} \left(\frac{\partial \Theta}{\partial q_i} - \Phi_i \right)^2 + V(q) = -\frac{\hbar}{i} \sum_i \frac{1}{2m_i} \frac{\partial^2 \Theta}{\partial q_i^2} \,. \tag{465}$$

The right- and left-hand sides of (465) are very different: $\hbar$, i, and the second derivative of Θ appear only on the right. If the right side is dropped, (465) becomes the Hamilton-Jacobi equation (455). Roughly speaking, therefore,

$$\psi \sim \exp\left(\frac{i}{\hbar} \times \text{classical action}\right) \qquad \hbar \to 0 \,, \tag{466}$$

which is the idea underlying the path integral.

It is now natural to consider a systematic expansion of Θ in powers of $\hbar$:

$$\Theta = S + \frac{\hbar}{i} S_1 + \left(\frac{\hbar}{i}\right)^2 S_2 + \dots \,, \tag{467}$$

where $S(q,t)$ is a solution of the Hamilton-Jacobi equation. According to (465), S will be a good approximation to Θ provided

$$|\partial S/\partial q_i|^2 \gg \hbar \, |\partial^2 S/\partial q_j^2| \,. \tag{468}$$

This inequality can be stated in a more meaningful way by considering the one-dimensional case, and defining the *local de Broglie wavelength* $\lambda\!\!\!^{-}(q)$ as

$$\frac{\hbar}{\lambda\!\!\!^{-}(q)} \equiv p(q) = \frac{\partial S}{\partial q} \,. \tag{469}$$

Then (468) becomes

$$\left|\frac{\partial \lambda\!\!\!^{-}}{\partial q}\right| \ll 1 \,. \tag{470}$$

That is, *the phase of the wave function is given by the classical action if the local wavelength $\lambda\!\!\!^{-}(q)$ changes but little in a distance of order the wavelength.*

An equation for the next term, S_1, is found by substituting (467) into the Schrödinger equation, and equating powers of $\hbar$:

$$\frac{\partial S_1}{\partial t} + \sum_k \frac{1}{2m_k}\left[2\left(\frac{\partial S}{\partial q_k} - \Phi_k\right)\frac{\partial S_1}{\partial q_k} + \frac{\partial^2 S}{\partial q_k^2}\right] = 0 \,. \tag{471}$$

This will produce a real function S_1 from the real action S in the regions of configuration space available to classical motions. When the higher-order terms, S_2, etc., are dropped, ψ is approximated by the *semiclassical wave function*[1]

$$\Psi_{\rm sc}(q,t) = e^{S_1(q,t)}\, e^{iS(q,t)/\hbar} = \sqrt{D(q,t)}\, e^{iS(q,t)/\hbar} \,. \tag{472}$$

In this approximation, the spatial probability distribution is

$$D(q,t) = |\Psi_{\rm sc}(q,t)|^2 = e^{2S_1(q,t)} \,, \tag{473}$$

which is independent of $\hbar$. The remarkable fact that the next-to-leading order term, $D(q,t)$, is $\hbar$-independent would seem to imply that it too is determined by classical mechanics. As we shall in the next subsection, that is indeed so.

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[1] Many authors refer to (472), and even the propagator $K_{\rm sc}$, as the WKB approximation. This is historically incorrect; we will only apply the name WKB to the stationary state one-dimensional case (see §4.5).

The relationship between $D(q,t)$ and $S(q,t)$ is opaque when expressed by (471), but will become clear when it is rewritten as follows:

$$\frac{\partial}{\partial t}e^{2S_1} + \sum_k \frac{\partial}{\partial q_k}\left[\frac{1}{m_k}\left(\frac{\partial S}{\partial q_k} - \Phi_k\right)e^{2S_1}\right] = 0\ . \tag{474}$$

The Schrödinger current i_k belonging to the wave function $\Psi_{\rm sc}$ is

$$i_k = \frac{1}{2m_k}\Psi^*_{\rm sc}\left(\frac{\hbar}{i}\frac{\partial}{\partial q_k} - \Phi_k\right)\Psi_{\rm sc} + \text{c.c.} = \frac{D}{m_k}\left(\frac{\partial S}{\partial q_k} - \Phi_k\right)\ . \tag{475}$$

Recalling (456) then gives the following intuitively appealing expression for the current,

$$i_k(q,t) = D(q,t)\,\dot{q}_k(t)\ , \tag{476}$$

where $\dot{q}_k$ is the velocity of a particle at the position $q_k(t)$ as it moves in accordance with the classical equations of motion. Eq. 474 is therefore

$$\frac{\partial D}{\partial t} + \sum_k \frac{\partial}{\partial q_k}(D\,\dot{q}_k) = 0\ , \tag{477}$$

i.e., *the continuity equation for a classical fluid of density $D(q,t)$ and local velocity $\dot{q}(t)$ moving through configuration space.* In short, (477) is the approximation to the quantum mechanical continuity equation for the flow of probability when a solution of the Schrödinger equation is replaced by the semiclassical wave function $\Psi_{\rm sc}$.

(c) The Semiclassical Propagator

The semiclassical wave function $\Psi_{\rm sc}(q,t)$ has intuitively pleasing properties. Nevertheless, given a wave function $\psi(q)$ at $t = 0$, it is not clear what conditions this initial data must satisfy if it is to be evolved in time in the form of $\Psi_{\rm sc}$. For example, if $\psi(q)$ is real, then the implication that $S(q, t = 0) = 0$ renders the Hamilton-Jacobi equation useless, and yet that is the equation that should supposedly be solved to evolve the semiclassical wave function. In this example, some more or less ad hoc method for assigning phases to such a real input would have to be devised.

This question does not arise, and compliance with the superposition principle is assured, if the the wave function is evolved with a properly constructed semiclassical propagator $K_{\rm sc}(b,a)$, so that time development is given by

$$\Psi(q;t) = \int d^f q'\, K_{\rm sc}(q,t;q',t')\,\Psi(q';t')\ . \tag{478}$$

The derivation of this approximate propagator is quite intricate, and therefore we first give the expression for $K_{\rm sc}$ and discuss its properties.

In §2.7(b) we found that the propagator for a free particle in one dimension is

$$K_0(b,a) = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}\ \exp\left(\frac{i}{\hbar}\,S^0(b,a)\right)\ , \tag{479}$$

where S^0 is *the classical action for a free particle.* Eq. 479 is exact. It turns out that this is a special case of a general but approximate result:

- In the limit $\hbar \to 0$, the propagator for an arbitrary system of particles has the form

$$K_{\rm sc}(b,a) = \sum_{\mathcal{P}_r} A_r(b,a)\ \exp\left\{ i\left(\frac{1}{\hbar} S_r(b,a) - \frac{\beta_r \pi}{2} \right) \right\}\ , \tag{480}$$

  where $S_r(b,a)$ is the classical action for the system in question when it follows the classically allowed path $\mathcal{P}_r$. In general, more than one classical path may connect b to a.

- The amplitude factor is known once the classical action $S_r(b,a)$ is known:[1]

$$A_r(b,a) = \left(\frac{i}{2\pi\hbar} \right)^{f/2} \sqrt{\det \frac{\partial^2 S_r(b,a)}{\partial q_{a,i} \partial q_{b,j}}}\ . \tag{481}$$

  The determinant in (481) is called the Van Vleck determinant $D_r(b,a)$. For each path, D_r and S_r satisfy the continuity equation (477).

- The integer β_r is called the Maslov index. It too is determined by the classical trajectories, and in particular, by the number of trajectory crossings encountered on the various paths. The $\hbar$-independent phase factor $\exp(-i\beta_r\pi/2)$ is essential, for if it is overlooked the wave function generated by (478) will not be continuous. (In this connection, recall Fig. 2.5.)

As it stands, $K_{\rm sc}$ can only produce an approximate wave function in classically allowed regions, so it cannot describe quantum tunneling. Techniques for analytically continuing the propagator into classically forbidden regions exist, but this is a difficult topic which we will not treat. A semiclassical technique for handling tunneling problems in one dimension is presented in §4.5, however.

The amplitude factor (481) is a classical quantity, so it should have a classical meaning. Indeed it does: $|A(b,a)|^2$ is the probability $P_{\rm cl}(q_b t_b; q_a t_a)$ for finding the configuration q_b at t_b for an ensemble of systems moving classically and known to have been in the configuration q_a at t_a. When an initial configuration $(q_a t_a)$ is specified, the uncertainty principle demands all momenta to be equally probable at that time. The normalization of this white momentum spectrum is given by (177):

$$|\langle p_a(t_a)|q_a(t)\rangle|^2 d^f p_a = \prod_i \left| \frac{e^{i p_{a,i} q_{a,i}/\hbar}}{(2\pi\hbar)^{1/2}} \right|^2 dp_{a,i} = \frac{d^f p_a}{(2\pi\hbar)^f}\ . \tag{482}$$

By assumption, each member of the ensemble moves classically from the initial condition $(q_a p_a)$, and will be in the interval $d^f q_b$ at t_b with a probability

$$P_{\rm cl}(q_b t_b; q_a t_a) d^f q_b = \frac{d^f p_a}{(2\pi\hbar)^f}\ . \tag{483}$$

In computing $d^f p_a / d^f q_b$, bear in mind that when the initial and final coordinates are specified, as they are here, the $p_{a,i}$ are functions of these coordinates and times. The ratio of differentials is therefore the Jacobian

$$\frac{d^f p_a}{d^f q_b} = \frac{\partial(p_{a,1}(b,a), \ldots, p_{a,f}(b,a))}{\partial(q_{b,1}, \ldots, q_{b,f})}\ , \tag{484}$$

[1] Note that because of (427) this agrees with (479).

where $p_{a,i}(b,a) = p_{a,i}(q_b t_b; q_a t_a)$. Using (448) for these initial momenta gives

$$\frac{\partial(p_{a,1}(b,a),\ldots,p_{a,f}(b,a))}{\partial(q_{b_b,1},\ldots,q_{b,f})} = (-1)^f \det \frac{\partial^2 S(b,a)}{\partial q_{b,i}\,\partial q_{a,j}} \,. \tag{485}$$

The quantum and classical probabilities, $|K(b,a)|^2$ and $P_{\rm cl}(b,a)$, therefore agree when the propagator is approximated by $K_{\rm sc}$ and there is only one path connecting b to a. If there is more than one, quantum mechanical interference terms will survive as $\hbar \to 0$ unless an average over rapidly oscillating terms is imposed by the resolution of an experiment.

The following subsection describes the steps that lead to $K_{\rm sc}(b,a)$ from the path integral: (i) The action for arbitrary paths is expanded about the classical path, and it is shown that only quadratic departures survive in the limit $\hbar \to 0$. The path integrals containing these quadratic terms form the factor $A_r(b,a)$. (ii) If the paths connecting a to b do not cross, an evaluation of the path integral expressing A_r can be sidestepped by requiring $K_{\rm sc}$ to satisfy the composition law for unitary transformations. (iii) If there are paths that cross, the path integral for the amplitude factors must be evaluated, which yields the phase shifts shown in (480).

Because only quadratic departures from the classical path survive the limit $\hbar \to 0$, the semiclassical approximation $K_{\rm sc}(b,a)$ is the exact propagator for all Hamiltonians that do not contain terms higher than quadratic in the canonical coordinates and momenta. Consequently, the classical action determines the propagators exactly for systems of arbitrary many harmonically coupled degrees of freedom; for particles subjected to constant forces; and for charged particles in a uniform magnetic field.

(d) Derivations

Our first objective is to find the $\hbar \to 0$ behavior of the path integral representing the propagator. The essential features can be seen in one dimension. As in §2.7(b), let $x(t)$ be an arbitrary path, $Q(t)$ the path prescribed by classical mechanics, $x(t) = Q(t) + y(t)$, and $S[x(t)]$ the action for the arbitrary path. Assume also that only one classical path exists for this particular case $a \to b$. As $Q(t)$ minimizes S,

$$S[Q(t)+y(t)] = S[Q(t)] + \int_{t_a}^{t_b} dt \left(\tfrac{1}{2} y^2 \frac{\delta^2 S}{\delta x^2} + \tfrac{1}{2}\dot{y}^2 \frac{\delta^2 S}{\delta \dot{y}^2} + y\dot{y} \frac{\delta^2 S}{\delta y \delta \dot{y}} \right) + \ldots \tag{486}$$

$$= S(b,a) + \int_{t_a}^{t_b} dt\, [a(t)\dot{y}^2 + b(t) y^2 + c(t) y\dot{y}] + \ldots \,, \tag{487}$$

where $+\ldots$ stands for terms of order y^3 and higher. In the free-particle case, $a = \frac{1}{2}m$ and all the other terms vanish, which is why the approximate answer is exact in this instance.

In consequence of (487), the propagator is

$$K(b,a) = \mathcal{A}(b,a)\, e^{iS(b,a)/\hbar} \,, \tag{488}$$

where $S(b,a)$ is the action for the classical trajectory, and $\mathcal{A}$ is the path integral

$$\mathcal{A}(b,a) = \int_{t_a, y=0}^{t_b, y=0} \mathcal{D}(y(t))\, \exp\left(\frac{i}{\hbar} \int_{t_a}^{t_b} dt\, [a(t)\dot{y}^2 + b(t) y^2 + c(t) y\dot{y}] + \ldots \right). \tag{489}$$

This should be compared to the corresponding expression for the free particle (Eq. 429). If the classical equation of motion allows several paths $Q_r(t)$ from a to b, then a sum on r is required, and the departures from each $Q_r(t)$ must be treated as in (489).

When the path integral is first approximated by κ steps of duration τ, as in Eq. 434, and dimensionless coordinates $\eta_\kappa = y_\kappa\sqrt{m/\hbar\tau}$ are introduced, it takes the form

$$\mathcal{A}(b,a) = \mathsf{Lim}\sqrt{m/\hbar\tau}\int_{-\infty}^{\infty} d^{\kappa-1}\eta \times \exp\left(f_2(\eta) + (\hbar\tau/m)^{\frac{1}{2}} f_3(\eta) + (\hbar\tau/m) f_4(\eta) + \ldots\right) , \quad (490)$$

where $f_n(\eta)$ comes from the terms of order y^n in (487), and is a polynomial of degree n in the variables $(\eta_1, \ldots, \eta_{\kappa-1})$. Hence all terms in the Lagrangian that are of higher order than quadratic are removed by the limit $\hbar \to 0$:

$$A(b,a) = \sqrt{m/\hbar}\,\mathsf{Lim}\,\tau^{-\frac{1}{2}}\int_{-\infty}^{\infty} d^{\kappa-1}\eta\ \exp[f_2(\eta)] . \quad (491)$$

The evaluation of the path integral (491) can be sidestepped when there is only one path connecting (a,b) by requiring the propagator to satisfy

$$K_{\rm sc}(x't';xt) = \int d\bar{x}\ K_{\rm sc}(x't';\bar{x}\bar{t})K_{\rm sc}(\bar{x}\bar{t};xt) \quad (492)$$

$$= \int d\bar{x}\ A(x';\bar{x})A(\bar{x};x)\exp\left(\frac{i}{\hbar}[S(x';\bar{x}) + S(\bar{x};x)]\right) , \quad (493)$$

which must hold for all $t < \bar{t} < t'$. (In Eq. 493 the time arguments have been suppressed.) The amplitude factors have a spatial variation that does not depend on $\hbar$. In contrast, the actions in the exponent are very large compared to $\hbar$ in the semiclassical limit, so the exponential varies rapidly as a function of $\bar{x}$. The integral can therefore be evaluated by the stationary phase method. The relevant formula is

$$\int dx\, g(x)e^{if(x)/\hbar} \simeq \sum_\alpha e^{if(x_\alpha)/\hbar}\int dx\, g(x)\ \exp\left[\tfrac{1}{2}i(x-x_\alpha)^2 f''(x_\alpha)/\hbar\right]$$

$$\simeq \sum_\alpha g(x_\alpha)\sqrt{\frac{2\pi i\hbar}{f''(x_\alpha)}}\ e^{if(x_\alpha)/\hbar} , \quad (494)$$

where x_α are the stationary phase points, $f'(x_\alpha) = 0$. According to (447) and (448), the stationary phase condition is

$$\frac{\partial}{\partial\bar{x}}[S(x';\bar{x}) + S(\bar{x};x)] = -p_0(x';\bar{x}) + p_0(\bar{x};x) = 0 , \quad (495)$$

where p_0 are momenta at the intermediate time $\bar{t}$. Eq. 495 has a simple meaning: a stationary phase point $x_0(\bar{t})$ is one where the momentum arriving and leaving that point are equal, so that the whole trajectory from (xt) to $(x't')$ is continuous at $\bar{t}$ (see Fig. 2.6).

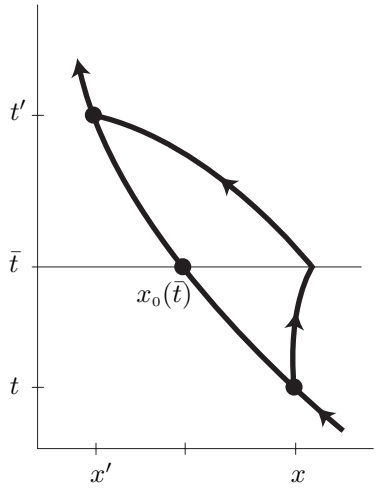

FIG. 2.6. The semiclassical propagators will only satisfy the composition law required by unitarity if the two trajectories join smoothly, which occurs at the stationary phase point $x_0(\bar{t})$.

This is required to permit the statement

$$S(x't;x_0\bar{t}) + S(x_0\bar{t};xt) = S(x't';xt) \ , \tag{496}$$

which must hold if (492) is to hold. In one dimension and for one given path there is only one point at any $\bar{t}$ at which the entering and leaving momenta are equal, and thus only one stationary phase point. Equation (493), in view of (494), requires the amplitude factors to satisfy

$$A(x';x) = \sqrt{2\pi i\hbar}\, A(x';x_0)A(x_0;x) \left(\frac{\partial^2}{\partial \bar{x}^2} [S(x';\bar{x}) + S(\bar{x};x)]_{\bar{x}=x_0} \right)^{-\frac{1}{2}} \ . \tag{497}$$

If (481) is to satisfy (497), the following must hold:

$$\frac{\partial^2 S(x';x)}{\partial x' \partial x} = -\frac{\partial^2 S(x';x_0)}{\partial x' \partial x_0} \, \frac{\partial^2 S(x_0;x)}{\partial x_0 \partial x} \left(\frac{\partial^2}{\partial x_0^2} [S(x';x_0) + S(x_0;x)] \right)^{-1} \ . \tag{498}$$

Now (495) is a relationship between (x, x', x_0) for given values of $(t, t', \bar{t}\,)$. Differentiation of this relationship with respect to x with x' held fixed gives

$$\left(\frac{\partial}{\partial x} \right)_{x'} [p_0(x_0;x) - p_0(x';x_0)] = \frac{\partial p_0(x_0;x)}{\partial x} + \frac{\partial x_0}{\partial x} \frac{\partial}{\partial x_0} [p_0(x_0;x) - p_0(x';x_0)] \ , \tag{499}$$

because $p_0(x';x_0)$ does not depend explicitly on x. Therefore the last factor in (498) is

$$\frac{\partial}{\partial x_0} [p_0(x';x_0) - p_0(x_0;x)] = \frac{\partial p_0(x_0;x)}{\partial x} \, \frac{\partial x}{\partial x_0} \ . \tag{500}$$

Furthermore, because of (496),

$$\frac{\partial^2 S(x';x_0)}{\partial x' \partial x_0} = \frac{\partial^2 S(x';x)}{\partial x' \partial x} \frac{\partial x}{\partial x_0} , \tag{501}$$

which with (500) establishes (498).

Two questions now arise: (i) How are more degrees of freedom to be handled? (ii) How are the phases of the propagators to be computed? The first question is answered by an exercise in Jacobian gymnastics, which can be found in the review by Berry and Mount.

The second question is much deeper, and we only offer a hint as to how it was first answered by Gutzwiller. Basically, the propagators for distinct classically allowed paths must be sown together to form a continuous function. If there are no paths between a and b that cross each other, the phases are those of the free particle propagator. Consider, however, the one-dimensional case where two paths connecting a to b cross at an intermediate point (x_c, t_c), which is called a point conjugate to a. The convolution (492) must hold for all times between t_a and t_b, and must, therefore, properly continue the phases generated by the two paths that converge on (x_c, t_c) from $t_c - \epsilon$ to $t_c + \epsilon$. This is done by returning to the path integral, in which only quadratic departures from classical paths survive when $\hbar \to 0$. The evaluation is then similar to that for free particles (see Eq. 436, etc.), though with a more complicated quadratic form in the fluctuations η_k, and hence a product of Gaussian integrals with different eigenvalues λ_k. In the free particle case, all the eigenvalues are positive, and give the same root of i; in the present case that is no longer true when there are conjugate points, and the Maslov index counts the number of eigenvalues that have the "wrong" sign and the extra phase factor as given by Eq. 380. An example of such a calculation can be found in §17 of Schulman's monograph. A powerful theory exists for multidimensional problems because the indices characterize the topology of the manifolds of orbits in configuration space.[1]

The proof that the Van Vleck determinant satisfies the continuity equation is sketched in Prob. 15.

2.9 Problems

1. Let A be a positive definite Hermitian operator. Show that for all $|u\rangle$ and $|v\rangle$,

$$|\langle u|A|v\rangle|^2 \geq \langle u|A|u\rangle\langle v|A|v\rangle .$$

Under what conditions does the equality hold?

2. Let $A(x)$ be an operator that depends on a continuous variable x. Define its derivative by

$$\frac{dA}{dx} \equiv A'(x) = \lim_{\epsilon \to 0} \frac{A(x+\epsilon) - A(x)}{\epsilon} .$$

If A has an inverse, show that

$$\frac{d}{dx} A^{-1} = -A^{-1} A' A^{-1} ;$$

and finally, if A and B both depend on x, that $d(AB)/dx = A'B + AB'$.

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[1] V.I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer (1980), pp. 442–445.

3. The object is to derive the density matrix $\rho_T = e^{-\beta H}/Z$ for a system in thermal equilibrium, where $\beta = 1/kT$. Show it results from maximizing the entropy for a fixed value of the internal energy $U = \mathrm{Tr}\,\rho_T H$.

4. Consider a system composed of two parts s and R, and let ρ be the density matrix for some state of the combined system. Show that for the subsystem to be in a pure state, ρ must have the form $P_s \otimes \rho_R$, where P_s is some projection operator onto the Hilbert space of s.

5. Confirm that Eq. 150 follows from Eq. 148. Show that the phase space representation of an arbitrary observable $\mathcal{A}(q,p)$ is given by Eq. 152.

6. Show that the uncertainty relation Eq. 203 becomes an equality when $|\phi\rangle$ is such that $|\phi_A\rangle$ and $|\phi_B\rangle$ are collinear, i.e., $|\phi_A\rangle = \lambda|\phi_B\rangle$, and $\lambda = \langle C\rangle/2i(\Delta B)^2$.

7. Show that the electrical charge and current densities, as given by (232) and (233), satisfy the continuity equation.

8. (a) By integrating the Heisenberg equations of motion for a free particle, derive Eq. 257. Show that this equation agrees with the evolution of the momentum distribution of a system of non-interacting particles in classical mechanics. Was this to be expected?

(b) Use Eq. 258 to compute the spreading of the following free particle wave packets confined at $t = 0$ to volumes of dimension R: (i) an electron with R the Bohr radius in hydrogen, and R the electron's Compton wavelength; (ii) an alpha particle for the same values of R, and the radius of the Pb nucleus; and (iii) and a golf ball with $R = 1\,\mu$m.

9. Show that the energy distribution of Eq. 270 leads to the exponential decay law if $\Gamma \ll E_0$.

10. Define $\Delta\boldsymbol{K} = (R-1)\boldsymbol{K}$ for the rotation R of any 3-vector $\boldsymbol{K}$, and let R_1 and R_2 be two infinitesimal rotations parametrized with $\delta\boldsymbol{\omega}_1$ and $\delta\boldsymbol{\omega}_2$. If $\Delta\boldsymbol{K}$ is the change induced in $\boldsymbol{K}$ by $R = R_2^{-1}R_1^{-1}R_2R_1$, show that to leading order

$$\Delta\boldsymbol{K} = -(\delta\boldsymbol{\omega}_1 \times \delta\boldsymbol{\omega}_2)\times\boldsymbol{K} \ .$$

11. (a) Let $\exp(i\Xi)$ be the phase factor in Eq. 349. Show that under a gauge transformation

$$\left(\boldsymbol{p}_n - \frac{e_n}{c}\boldsymbol{A}_n\right)\psi \to e^{i\Xi}\left(\boldsymbol{p}_n - \frac{e_n}{c}\boldsymbol{A}_n\right)\psi \ ,$$

where $\boldsymbol{A}_n = \boldsymbol{A}(\boldsymbol{r}_n, t)$, and $\boldsymbol{A}'_n$ is given by (345). Show that the current as defined in (351) is gauge invariant, whereas (227) is not.

(b) Let $\boldsymbol{x}_n$ be the coordinate operator for a particle whose motion is governed by the Hamiltonian (348). Show that $\boldsymbol{v}_n = \dot{\boldsymbol{x}}_n$, where $\boldsymbol{v}_n$ is given by (350).

(c) Show that the probability current of Eq. 351 satisfies the continuity equation in configuration space (Eq. 226).

12. Derive Green's function for a free particle in one dimension (Eq. 390) by (i) evaluating the $d = 1$ counterpart of (386); and (ii) by directly solving the inhomogeneous Schrödinger equation.

13. This problem concerns the following important special case of the BCH theorem: If A and B are two operators that do not commute with each other but which both commute with $[A, B]$, they satisfy

$$e^{A+B} = e^A\, e^B\, e^{-\frac{1}{2}[A,B]} \ .$$

(a) To prove this, first show that $[B, e^{xA}] = e^{xA}[B, A]x$. Next, define $G(x) = e^{xA}e^{xB}$, and show that

$$\frac{dG}{dx} = (A + B + [A, B]x)G \ .$$

Integrate this to obtain the desired result.

(b) More generally, show that for arbitrary A and B

$$\lim_{\alpha,\beta\to 0} e^{\alpha A}\ e^{\beta B} = e^{\alpha A+\beta B+\frac{1}{2}\alpha\beta[A,B]+X} \ ,$$

where X is of higher order in α, β.

14. Let D_κ be the determinant of the κ-dimensional matrix (438). Show that $D_\kappa = 2D_{\kappa-1} - D_{\kappa-2}$, and that (443) is the solution of this recursion relation.

15. To prove that the Van Vleck determinant D satisfies the continuity equation, show first that for any non-singular matrix A with elements a_{ij} that depend on the parameter z,

$$\frac{\partial D}{\partial z} = D\sum_{ij}(A^{-1})_{ji}\frac{\partial a_{ij}}{\partial z} \ .$$

Calling $a_{ij} = \partial^2 S/\partial q_i \partial q'_j$, show that the continuity equation follows in virtue of the Hamilton-Jacobi equation.

Endnotes

For mathematically respectable presentations of quantum mechanics, see T.F. Jordan, *Linear Operators for Quantum Mechanics,* Wiley (1969); W. Thirring, *A Course in Mathematical Physics, v.3, Quantum Mechanics of Atoms and Molecules*, Springer (1981).

The question of whether the quantum state should be associated with individual systems, or with ensemble of systems, and the related issue of how probabilities should be introduced into quantum mechanics, are discussed by W. Heisenberg, *Physics and Philosophy*, Harper (1962); and A. Shimony, *Search for a Naturalistic World View*, Vol. II, Cambridge University Press (1993); A. Shimony in *Epistemological and Experimental Perspectives on Quantum Physics,* D. Greenberger et al. (eds.), Kluwer (1999). This question has been analyzed in mathematical terms by E. Farhi, J. Goldstone and S. Gutmann, *Ann. Phys.* **192**, 368 (1989); and S. Gutmann, *Phys. Rev. A* **52**, 3560 (1995). They formulate the postulates in terms of the state $|\psi\rangle$ of an individual system $\mathcal{S}$; introduce the state $|\psi\rangle^\infty$ of an infinite number of copies of $\mathcal{S}$, i.e., $|\psi\rangle \otimes |\psi\rangle \otimes \ldots$, and a frequency operator $F(a_i)$ for the eigenvalue a_i of the observable A pertaining to an individual $\mathcal{S}$; and show that $|\psi\rangle^\infty$ is an eigenstate of $F(a_i)$ with eigenvalue $|\langle a_i|\psi\rangle|^2$.

Probabilities having the quantum mechanical interference properties are derived by Y.F. Orlov from the absence, in principle, of any algorithm that determines the outcome of measurements: *Phys. Rev. Lett.* **82**, 243 (1999); *Ann. Phys.* **234**, 245 (1994).

Because quantum states are in general not pure, and also because the state space is a ray space, a formulation that treats the density matrix as basic, rather than kets, has considerable attraction. For such a formulation see R. Balian, *Am. J. Phys.* **57**, 1019 (1989); and *From Microphysics to Macrophysics*, Vol. 1, Springer (1991), chapter 2.

The path integral is treated in a mathematically serious manner in B. Simon, *Functional Integration in Quantum Physics*, Academic Press (1979). The classic reference on path integrals is R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw Hill (1965).

Our treatment of semiclassical quantum mechanics draws on M.V. Berry and K.E. Mount, *Rep. Prog. Phys.* **35**, 315-397 (1972); M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Springer (1990); E.J. Heller, in *The Physics and Chemistry of Wave*

Packets, J.A. Yeazell and T. Uzer (eds.), Wiley (2000); W.H. Miller, *Adv. Chem. Phys.* **25**, 69-177 (1974); W. Pauli, *Pauli Lectures in Physics,* Vol. 6, C.P. Enz (ed.), MIT Press (1973); L.S. Schulman, *Techniques and Applications of Path Integration*, Wiley (1981); and H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics*, 2nd. ed., World Scientific (1995). An extensive and remarkable bibliography on semiclassical quantum mechanics and related topics is provided by M.C. Gutzwiller, *Am. J. Phys.* **66**, 304 (1998). The connection between mechanics and geometrical optics is treated in M. Born and E. Wolf, *Principles of Optics*, Pergamon (1959).