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Preface

World Scientific Publishing Company recently published my book entitled *Introduction to Modern Physics: Theoretical Foundations*. The book is aimed at the very best students, with a goal of exposing them to the foundations and frontiers of today's physics. Typically, students have to wade through several courses to see many of these topics, and I wanted them to have some idea of where they were going, and how things fit together, as they went along. Hopefully, they will then see more inter-relationships, and get more original insights, as they progress. The book assumes the reader has had a good one-year, calculus-based freshman physics course, along with a good one-year course in calculus. While it is assumed that mathematical skills will continue to develop, several appendices are included to bring the reader up to speed on any additional mathematics required at the outset. With very few exceptions, the reader should then find the material to be self-contained. Many problems are included, some for each chapter. Although the book is designed so that one can, in principle, read and follow the text without doing any of the problems, the reader is strongly urged to attempt as many of them as possible in order to obtain some confidence in his or her understanding of the basics of modern physics and to hone working skills.

After completing that book, it occurred to me that a second volume could be prepared that would significantly extend the coverage, while furthering the stated goals. The ground rules would be that anything covered in the text and appendices of the first volume would be fair game, while anything covered in the problems would first be re-summarized. Those few results quoted without proof in Vol. I would now be derived. The topics chosen would be those of wide applicability in all areas of physics. Again, an important goal would be to keep the entire coverage self-contained. The

present book is the outcome of those musings. All of the material in this book is taken from course lectures given over the years by the author at either Stanford University or the College of William and Mary.

Quantum mechanics is first reformulated in abstract Hilbert space, which allows one to focus on the general structure of the theory. The book then covers the following topics: angular momentum, scattering theory, lagrangian field theory, symmetries, Feynman rules, quantum electrodynamics, path integrals, and canonical transformations for quantum systems. Several appendices are included with important details. When finished, the reader should have an elementary working knowledge in the principal areas of theoretical physics of the twentieth century. With this overview in hand, development in depth and reach in these areas can then be obtained from more advanced physics courses.

I was again delighted when World Scientific Publishing Company, which had done an exceptional job with four of my previous books, showed enthusiasm for publishing this new one. I would like to thank Dr. K. K. Phua, Executive Chairman of World Scientific Publishing Company, and my editor Ms. Lakshmi Narayanan, for their help and support on this project. I am greatly indebted to my colleagues Paolo Amore and Alfredo Aranda for their reading of the manuscript.

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Chapter 1

Introduction

The goal of this book is to provide an extension of the previous book *Introduction to Modern Physics: Theoretical Foundations*, refered to as Vol. I. That volume develops the underlying concepts in twentieth-century physics: quantum mechanics, special relativity, and general relativity. Included in it are applications in atomic, nuclear, particle, and condensed matter physics. It is assumed in Vol. I that readers have had a good calculus-based introductory physics course together with a good course in calculus. Several appendices then provide sufficient background so that, with very few exceptions, the presentation is self-contained. Many of the topics covered in that work are more advanced than in the usual introductory modern physics books. It was the author's intention to provide the best students with an overview of the subject, so that they are aware of the overall picture and can see how things fit together as they progress.

As projected in Vol. I, it is now assumed that mathematical skills have continued to develop. In this volume, readers are expected to be familiar with multi-variable calculus, in particular, with multiple integrals. It is also assumed that readers have some familiarity with the essentials of linear algebra. An appendix is included here on functions of a complex variable, since complex integration plays a key role in the analysis. The ground rules now are that anything covered in the text and appendices in Vol. I is assumed to be mastered, while anything covered in the problems in Vol. I will be re-summarized. Within this framework, readers should again find Vol. II to be self-contained.

There are over 175 problems in this book, some after each chapter and appendix. The problems are not meant to baffle the reader, but rather to enhance the coverage and to provide exercises on working skills. The problems for the most part are not difficult, and in most cases the steps

are clearly laid out. Those problems that may involve somewhat more algebra are so noted. The reader is urged to attempt as many problems as possible in order to obtain some confidence in his or her understanding of the framework of modern theoretical physics.

In chapter 2 we revisit quantum mechanics and reformulate the theory in terms of linear hermitian operators acting in an abstract Hilbert space. Once we know how to compute inner products, and have the completeness relation, we understand the essentials of operating in this space. The basic elements of measurement theory are also covered. We are then able to present quantum mechanics in terms of a set of postulates within this framework. The quantum fields of Vol. I are operators acting in the abstract many-particle Hilbert space.

Chapter 3 is devoted to the quantum theory of angular momentum, and this subject is covered in some depth. There are a variety of motivations here: this theory governs the behavior of any isolated, finite quantum mechanical system and lies at the heart of most of the applications in Vol. I;[1] it provides a detailed illustration of the consequences of a continuous symmetry in quantum mechanics, in this case the very deep symmetry of the isotropy of space; furthermore, it provides an extensive introduction to the theory of Lie groups, here the special unitary group in two dimensions SU(2), which finds wide applicability in internal symmetries. An appendix explores the use of angular momentum theory in the multipole analysis of the radiation field, which is applicable to transitions in any finite quantum mechanical system.

Chapter 4 is devoted to scattering theory. The Schrödinger equation is solved in terms of a time-development operator in the abstract Hilbert space, and the scattering operator is identified. The interaction is turned on and off "adiabatically", which allows a simple construction of initial and final states, and the S-matrix elements then follow immediately. Although inappropriate for developing a covariant scattering analysis, the time integrations in the scattering operator can be explicitly performed and contact made with time-independent scattering theory. It is shown how adiabatic damping puts the correct boundary conditions into the propagators. A general expression is derived for the quantum mechanical transition rate. Non-relativistic scattering from a static potential provides a nice example of the time-independent analysis. If the time is left in the scattering operator, one has a basis for the subsequent analysis in terms of Feynman

[1] For example, here we validate the "vector model" used there.

diagrams and Feynman rules. The tools developed in this chapter allow one to analyze any scattering or reaction process in quantum mechanics.

Lagrangian field theory provides the dynamical framework for a consistent, covariant, quantum mechanical description of many interacting particles, and this is the topic in chapter 4. We first review classical lagrangian particle mechanics, and then classical lagrangian continuum mechanics, using our paradigm of the transverse planar oscillations of a string. The string mechanics can be expressed in terms of "two-vectors" (x, ict) where c is the sound velocity in the string. We then discuss the quantization of these classical mechanical systems obtained by imposing canonical quantization relations on the operators in the abstract Hilbert space.

The appending of two additional spatial dimensions to obtain four-vectors $(\mathbf{x}, ict)$, where c is now the speed of light, leads immediately to a covariant, continuum lagrangian mechanics for a scalar field in Minkowski space, which is then quantized with the same procedure used for the string. We develop a covariant, continuum lagrangian mechanics for the Dirac field, and discuss how anticommutation relations must be imposed when quantizing in this case. A general expression is derived for the energy-momentum tensor, and Noether's theorem is proven, which states that for every continuous symmetry of the lagrangian density there is an associated conserved current. A full appendix is dedicated to the lagrangian field theory of the electromagnetic field.

Symmetries play a central role in developing covariant lagrangian densities for various interacting systems, and chapter 6 is devoted to symmetries. The discussion starts with spatial rotations and the internal symmetry of isospin, and it builds on the analysis of SU(2) in chapter 3. Here isospin is developed in terms of global SU(2) transformations of the nucleon field $\psi = (\psi_p, \psi_n)$. The internal symmetry is generalized to SU(3) within the framework of the Sakata model with a baryon field $\psi = (\psi_p, \psi_n, \psi_\Lambda)$.[2]

It is also shown in chapter 6 how the imposition of invariance under local phase transformations of the charged Dirac field, where the transformation parameter depends on the space-time point x, necessitates the introduction of a photon (gauge) field $A_\mu(x)$ and leads to quantum electrodynamics (QED), the most accurate theory known. Yang-Mills theory, which extends this idea to invariance under local internal symmetry transformations of the Dirac field, and necessitates the introduction of corresponding gauge bosons, is developed in detail. These gauge bosons must be massless, and to

[2]Wigner's supermultiplet theory based on internal SU(4) transformations of the nucleon field $\psi = (\psi_{p\uparrow}, \psi_{p\downarrow}, \psi_{n\uparrow}, \psi_{n\downarrow})$ is also touched on.

understand the very successful physical application of Yang-Mills theories, it is necessary to understand how mass is generated in relativistic quantum field theories.[3]

We do this within the framework of the σ-model, a very simple model which has had a profound effect on the development of modern physics. A massless Dirac field has an additional chiral invariance under a global transformation that also mixes the components of the Dirac field. The corresponding conserved axial-vector current, which augments the conserved vector current arising from global isospin invariance, corresponds closely to what is observed experimentally in the weak interactions. The σ-model extends the massless Dirac lagrangian through a chiral-invariant interaction with a pion and scalar field $(\boldsymbol{\pi}, \sigma)$. A choice of shape of the chiral-invariant meson potential $\mathcal{V}(\boldsymbol{\pi}^2+\sigma^2)$ then leads to a vacuum expectation value for the scalar field that gives rise to a mass for the Dirac particle while maintaining chiral invariance of the lagrangian. This *spontaneous symmetry breaking* illustrates how observed states do not necessarily reflect the symmetry of the underlying lagrangian. Generating mass through the expectation value of a scalar field, in one way or another, now underlies most modern theories of particle interactions.[4]

The most fundamental symmetry in nature is Lorentz invariance. One must obtain the same physics in any Lorentz frame. The Lorentz transformation properties of the scalar and Dirac fields are detailed in an appendix. Some very useful tools are provided in another appendix devoted to the irreducible representations of SU(n).

Chapter 7 is concerned with the derivation of the Feynman rules, and to focus on the method, they are developed for the simplest theory of a Dirac particle interacting with a neutral, massive, scalar field. Wick's theorem is proven. This allows one to convert a time-ordered product of fields in the interaction picture, where the time dependence is that of free fields, into a normal-ordered product where the destruction operators sit to the right of the creation operators for all times. It is the time-ordered product that occurs naturally in the scattering operator, and it is the normal-ordered product from which it is straightforward to compute any required matrix elements. Wick's theorem introduces the vacuum expectation value

[3]Both quantum chromodynamics (QCD) and the Standard Model of electroweak interactions are Yang-Mills theories built on internal symmetry groups, the former on an internal color $SU(3)_C$ symmetry and the latter on an internal weak $SU(2)_W \bigotimes U(1)_W$.

[4]In the Standard Model, it provides the basis for the "Higgs mechanism" (see, for example, [Walecka (2004)]).

of the time-ordered product of pairs of interaction-picture fields— these are the *Feynman propagators*. An appendix provides a thorough discussion of these Green's functions, as well as other singular functions, for the scalar, Dirac, and electromagnetic fields.[5] The lowest-order scattering amplitudes, self-energies, and vacuum amplitude are all calculated for the Dirac-scalar theory, and then interpreted in terms of Feynman diagrams and Feynman rules. The cancellation of the disconnected diagrams is demonstrated in this chapter, as is the requisite procedure for mass renormalization.

In chapter 8 these techniques are applied to a theory with immediate experimental implications. That theory is quantum electrodynamics (QED), where the fine-structure constant $\alpha = e^2/4\pi\hbar c\varepsilon_0 = 1/137.04$ provides a meaningful dimensionless expansion parameter. The point of departure here is the derived QED hamiltonian in the Coulomb gauge, where $\boldsymbol{\nabla}\cdot\mathbf{A}(x) = 0$ and there is a one-to-one correspondence between the degrees of freedom in the vector potential and transverse photons. The interaction of the electron current and vector potential is combined with the instantaneous Coulomb interaction to produce a photon propagator, and then conservation of the interaction-picture current is invoked to reduce this to an effective photon propagator with a Fourier transform in Minkowski space of $\tilde{D}_{\mu\nu}(q) = \delta_{\mu\nu}/q^2$. One thereby recovers covariance and gauge invariance in the electromagnetic interaction.

The steps leading from an S-matrix element to a cross section are covered in detail in two examples, $\mu^- + e^- \to \mu^- + e^-$ and $e^+ + e^- \to \mu^+ + \mu^-$. Expressions are obtained in the center-of-momentum (C-M) frame that are exact to $O(\alpha^2)$. The scattering operator is extended to include an interaction with a specified external field, and the lowest-order amplitudes for bremsstrahlung and pair production are obtained. The Feynman diagrams and Feynman rules in these examples serve to provide us with the Feynman diagrams and Feynman rules for QED.

Chapter 9 presents an introduction to the calculation of various virtual processes in relativistic quantum field theory, and again, to keep close contact with experiment, we focus on QED. Calculations of the $O(\alpha)$ corrections to the scattering amplitude for an electron in an external field provide an introduction to the relevant lowest-order "loop" contributions, where there is an integral over one virtual four-momentum. The insertions here are characterized through the electron self-energy, vertex modification, and vacuum polarization (photon self-energy) diagrams.

[5] The neutral, massive vector meson field is covered in the problems.

Dimensional regularization, detailed in an appendix, serves as a technique that gives mathematical meaning to originally ill-defined integrals. Here one works in the complex n-plane, where n is the dimension, and any potential singularity is then isolated at the point $n \to 4$. The contribution of each of the above diagrams is cast into a general form that isolates such singular pieces and leaves additional well-defined convergent expressions.

Some care must be taken with the contribution of the self-energy insertions on the external legs ("wavefunction renormalization"), and we do so. It is then shown how Ward's identity, which relates the electron self-energy and vertex insertion, leads to a *cancellation* in the scattering amplitude of the singular parts of these insertions. Vacuum polarization then leads to a shielding of the charge in QED and to charge renormalization. The two remaining singular terms in the theory are removed by mass and charge renormalization, and if the scattering amplitude is consistently expressed in terms of the renormalized mass and charge (m, e) one is left with finite, calculable, $O(\alpha)$ corrections to the scattering amplitude. The Schwinger term in the anomalous magnetic moment of the electron is calculated here. Higher-order corrections are summarized in terms of Dyson's and Ward's equations, and it is demonstrated through Ward's identities how the multiplicative renormalizability of QED holds to all orders.

With the techniques developed in chapter 9, one has the tools with which to examine loop contributions in any relativistic quantum field theory.

Chapter 10 is on path integrals. There are many reasons for becoming familiar with the techniques here, which underly much of what now goes on in theoretical physics, for example: this approach provides an alternative to canonical quantization, which, with derivative couplings, can become prohibitively difficult; here one deals entirely with classical quantities, in particular the classical lagrangian and classical action; and the classical limit $\hbar \to 0$ leads immediately to Hamilton's principle of stationary action.

We start from the analysis of a non-relativistic particle moving in a potential in one dimension and show how the quantum mechanical transition amplitude can be exactly expressed as an integral over all possible paths between the initial and final space-time points.[6] We then make the transition to a system with many degrees of freedom, and then to field theory.

The addition of an arbitrary source term, together with the crucial theorem of Abers and Lee, allows one to construct the generating functional as a ratio of two path integrals, one a transition amplitude containing the

[6]It is shown in a problem how the partition function of statistical mechanics in the microcanonical ensemble can also be expressed as a path integral.

source and the second a vacuum-vacuum amplitude without it. The connected Green's functions can then be determined from the generating functional by functional differentiation with respect to the source, as detailed here. The generating functional is calculated for the free scalar field using gaussian integration, and it is shown how the Feynman propagator and Wick's theorem are reproduced in this case. The treatment of the Dirac field necessitates the introduction of Grassmann variables, which are anticommuting c-numbers. The generating functional is computed for the free Dirac field, and the Feynman propagator and Wick's theorem again recovered. It is shown how to include interactions and express the full generating functional in terms of those already computed.

An appendix describes how one uses the Faddeev-Popov method in a gauge theory, at least for QED, to factor the measure in the path integral into one part that is an integral over all gauge functions and a second part that is gauge invariant. With a gauge-invariant action, the path integral over the gauge functions then factors and cancels in the generating functional ratio. It is shown how the accompanying Faddeev-Popov determinant can be expressed in terms of ghost fields, which also factor and disappear from the generating functional in the case of QED. The generating functional for the free electromagnetic field is calculated here.

Although abbreviated, the discussion in chapter 10 should allow one to use path integrals with some facility, and to read with some understanding material that starts from path integrals.

The final chapter 11 deals with canonical transformations for quantum systems. Chapter 11 of Vol. I provides an introduction to the properties of superfluid Bose systems and superconducting Fermi systems. In both cases, in order to obtain a theoretical description of the properties of the quantum fluids, it is necessary to include interactions. A technique that has proven invaluable for the treatment of such systems is that of canonical transformations. Here one makes use of the fact that the properties of the creation and destruction operators follow entirely from the canonical (anti)commutation relations in the abstract Hilbert space. By introducing new "quasiparticle" operators that are linear combinations of the original operators, and that preserve these (anti)commutation relations, one is able to obtain exact descriptions of some interacting systems, both in model problems and in a starting hamiltonian.

The problem of a weakly interacting Bose gas with a repulsive interaction between the particles is solved with the Bogoliubov transformation. A phonon spectrum is obtained for the many-body system, which, as shown

in Vol. I, allows one to understand superfluidity. Motivated by the Cooper pairs obtained in Vol. I, a Fermi system with an attractive interaction between those particles at the Fermi surface is analyzed with the Bogoliubov-Valatin transformation. The very successful BCS theory of superconductivity is obtained in the case that the residual quasiparticle interactions can be neglected.

A problem takes the reader through the Bloch-Nordsieck transformation, which examines the quantized electromagnetic field interacting with a specified, time-independent current source. A key insight into the infrared problem in QED is thereby obtained. A second problem guides the reader through the analysis of a quantized, massive, neutral scalar field interacting with a classical, specified, time-independent source. The result is an exact derivation of the Yukawa interaction of nuclear physics.

This book is designed to further the goals of Vol. I and to build on the foundation laid there. Volume II covers in more depth those topics that form the essential framework of modern theoretical physics.[7] Readers should now be in a position to go on to more advanced texts, such as [Bjorken and Drell (1964); Bjorken and Drell (1965); Schiff (1968); Itzykson and Zuber(1980); Cheng and Li (1984); Donoghue, Golowich, and Holstein (1993); Merzbacher (1998); Fetter and Walecka (2003a); Walecka (2004); Banks (2008)], with a deeper sense of appreciation and understanding.

Modern theoretical physics provides a basic understanding of the physical world and serves as a platform for future developments. When finished with this book, readers should have an elementary working knowledge in the principal areas of theoretical physics of the twentieth-century.

[7]The author considered also including in Vol. II a chapter on solutions to the Einstein field equations in general relativity; however, given the existence of [Walecka (2007)], it was deemed sufficient to simply refer readers to that book.

Chapter 2

Quantum Mechanics (Revisited)

In this chapter we formalize some of the analysis of quantum mechanics in Vol. I, which will allow us to focus on the general structure of the theory. We start the discussion with a review of linear vector spaces.

2.1 Linear Vector Spaces

Consider the ordinary three-dimensional linear vector space in which we live.

2.1.1 *Three-Dimensional Vectors*

Introduce an orthonormal set of basis vectors $\mathbf{e}_i$ with $i = 1, 2, 3$ satisfying

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \qquad ; \ (i, j) = 1, 2, 3 \tag{2.1}$$

An arbitrary vector $\mathbf{v}$ is a physical quantity that has a direction and length in this space. It can be expanded in the basis $\mathbf{e}_i$ according to

$$\mathbf{v} = \sum_{i=1}^{3} v_i \mathbf{e}_i \qquad ; \ v_i = \mathbf{e}_i \cdot \mathbf{v} \tag{2.2}$$

$\mathbf{v}$ can now be characterized by its components (v_1, v_2, v_3) in this basis.[1] Vectors have the following properties:

(1) Addition of vectors, and multiplication of a vector by a constant, are

[1] This characterization will be denoted by $\mathbf{v} : (v_1, v_2, v_3)$.

expressed in terms of the components by

$$\begin{aligned} \mathbf{a}+\mathbf{b}: &\ (a_1+b_1, a_2+b_2, a_3+b_3) \\ \gamma\mathbf{a}: &\ (\gamma a_1, \gamma a_2, \gamma a_3) \qquad ;\ \text{linear space} \end{aligned} \tag{2.3}$$

These properties characterize a *linear space*;

(2) The dot product, or inner product, of two vectors is defined by

$$\mathbf{a}\cdot\mathbf{b} \equiv a_1b_1 + a_2b_2 + a_3b_3 \qquad ;\ \text{dot product} \tag{2.4}$$

The *length* of the vector is then determined by

$$|\mathbf{v}| = \sqrt{\mathbf{v}^2} = \sqrt{\mathbf{v}\cdot\mathbf{v}} = (v_1^2+v_2^2+v_3^2)^{1/2} \qquad ;\ \text{length} \tag{2.5}$$

One says that there is an *inner-product norm* in the space.

(3) Suppose one goes to a new orthonormal basis $\boldsymbol{\alpha}_i$ where the vector $\mathbf{v}$ has the components $\mathbf{v}: (\bar{v}_1, \bar{v}_2, \bar{v}_3)$. Then the components are evidently related by

$$\begin{aligned} \mathbf{v} &= \sum_{i=1}^{3} v_i\mathbf{e}_i = \sum_{i=1}^{3} \bar{v}_i\boldsymbol{\alpha}_i \\ \Rightarrow \qquad v_i &= \sum_{j=1}^{3} \bar{v}_j(\mathbf{e}_i\cdot\boldsymbol{\alpha}_j) = \sum_{j=1}^{3} \bar{v}_j[\boldsymbol{\alpha}_j]_i \end{aligned} \tag{2.6}$$

2.1.2 *n-Dimensions*

These arguments are readily extended to n-dimensions by simply increasing the number of components

$$\mathbf{v}: \ (v_1, v_2, v_3, \cdots, v_n) \qquad ;\ n\text{-dimensions} \tag{2.7}$$

The extension to *complex vectors* is accomplished through the use of the linear multiplication property with a complex γ. The positive-definite norm is then correspondingly defined through $|\mathbf{v}|^2 \equiv \mathbf{v}^\star\cdot\mathbf{v}$,

$$\begin{aligned} \gamma\mathbf{v}: &\quad (\gamma v_1, \gamma v_2, \gamma v_3, \cdots, \gamma v_n) \qquad ;\ \text{complex vectors} \\ |\mathbf{v}|^2 &\equiv \mathbf{v}^\star\cdot\mathbf{v} = |v_1|^2 + |v_2|^2 + \cdots + |v_n|^2 \end{aligned} \tag{2.8}$$

2.2 Hilbert Space

The notion of a *Hilbert space* involves the generalization of these concepts to a space with an infinite number of dimensions. Let us start with an example.

2.2.1 *Example*

Recall the set of plane waves in one spatial dimension in an interval of length L satisfying periodic boundary conditions

$$\phi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x} \quad ; \; k_n = \frac{2\pi n}{L} \quad ; \; n = 0, \pm 1, \pm 2, \cdots \quad ; \quad \text{basis vectors} \tag{2.9}$$

These will be referred to as the *basis vectors*. They are orthonormal and satisfy

$$\begin{aligned} \int_0^L dx\, \phi_m^\star(x)\phi_n(x) &= \delta_{mn} \quad ; \text{ orthonormal} \\ &\equiv \langle \phi_m | \phi_n \rangle \quad ; \text{ inner product} \end{aligned} \tag{2.10}$$

This relation allows us to define the *inner product* of two basis vectors, denoted in the second line by $\langle \phi_m | \phi_n \rangle$,[2] and the positive-definite *inner-product norm* of the basis vectors is then given by

$$|\phi_n|^2 = \langle \phi_n | \phi_n \rangle = \int_0^L dx\, |\phi_n(x)|^2 \quad ; \; (\text{“length”})^2 \tag{2.11}$$

An arbitrary function $\psi(x)$ can be expanded in this basis according to

$$\psi(x) = \sum_{n=-\infty}^{\infty} c_n \phi_n(x) \quad ; \text{ expansion in complete set} \tag{2.12}$$

This is, after all, just a complex Fourier series. The orthonormality of the basis vectors allows one to solve for the coefficients c_n

$$c_n = \langle \phi_n | \psi \rangle = \int_0^L dx\, \phi_n^\star(x)\psi(x) \tag{2.13}$$

[2]The notation, and most of the analysis in this chapter, is due to Dirac [Dirac (1947)].

Any piecewise continuous function can actually be expanded in this set, and the basis functions are *complete* in the sense that[3]

$$\text{Lim}_{N\to\infty} \int_0^L dx \left| \psi(x) - \sum_{n=-N}^{N} c_n \phi_n(x) \right|^2 = 0 \qquad ; \text{ completeness} \quad (2.14)$$

Just as with an ordinary vector, the function $\psi(x)$ can now be characterized by the expansion coefficients c_n

$$\begin{aligned} \psi(x) \ &: (c_{-\infty}, \cdots, c_{-1}, c_0, c_1, \cdots, c_\infty) \\ \text{or;} \qquad \psi \ &: \{c_n\} \end{aligned} \quad (2.15)$$

Addition of functions and multiplication by constants are defined in terms of the coefficients by

$$\begin{aligned} \psi^{(1)} + \psi^{(2)} \ &: \{c_n^{(1)} + c_n^{(2)}\} \\ \gamma\psi \ &: \{\gamma c_n\} \qquad\qquad ; \text{ linear space} \end{aligned} \quad (2.16)$$

This function space is again a *linear space*. The norm of ψ is given by

$$|\psi|^2 = \langle\psi|\psi\rangle = \int_0^L dx\, |\psi(x)|^2 = \sum_{n=-\infty}^{\infty} |c_n|^2 \qquad ; \text{ (norm)}^2 \quad (2.17)$$

which, in the case of Fourier series, is just Parseval's theorem.

2.2.2 *Definition*

The function $\psi(x)$ in Eq. (2.17) is said to be square-integrable. The set of all square-integrable functions ($\mathcal{L}^2$) forms a *Hilbert space*. Mathematicians define a Hilbert space as follows:

(1) It is a linear space;
(2) There is an inner-product norm;
(3) The space is complete in the sense that every Cauchy sequence converges to an element in the space.

The above analysis demonstrates, through the expansion coefficients c_n, the isomorphism between the space of all square-integrable functions ($\mathcal{L}^2$) and the ordinary infinite-dimensional complex linear vector space (l^2) discussed at the beginning of this section.

[3]This is all the completeness we will need for the physics in this volume.

2.2.3 *Relation to Linear Vector Space*

A more direct analogy to the infinite-dimensional complex linear vector space (l^2) is obtained through the following identification

$$v_i \to \psi_x \qquad ;\ \text{coordinate space} \tag{2.18}$$

We now use the coordinate x as a subscript, and we note that it is here a *continuous* index. The square of the norm then becomes

$$\sum_i v_i^\star v_i \to \sum_x \psi_x^\star \psi_x \equiv \int dx\, \psi^\star(x)\psi(x) \tag{2.19}$$

The sum over the continuous index has here been appropriately defined through a familiar integral. With this notation, the starting expansion in Eq. (2.12) takes the form

$$\psi_x = \sum_{n=-\infty}^{\infty} c_n [\phi_n]_x \tag{2.20}$$

2.2.4 *Abstract State Vector*

Equation (2.20) can be interpreted in the following manner:

> *This is just one component of the abstract vector relation*

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle \qquad ;\ \textit{abstract vector relation} \tag{2.21}$$

> *The quantity $|\psi\rangle$ is now interpreted as a vector in an infinite-dimensional, abstract Hilbert space. It can be given a concrete representation through the component form in Eqs. (2.20) and (2.12), using the particular set of basis vectors in Eqs. (2.9).*

As before, one solves for the expansion coefficients c_n by simply using the orthonormality of the basis vectors in Eq. (2.10)

$$c_n = \langle \phi_n | \psi \rangle = \sum_x [\phi_n]_x^\star \psi_x = \int dx\, \phi_n^\star(x)\psi(x) \tag{2.22}$$

2.3 Linear Hermitian Operators

Consider an operator L in Hilbert space. Given $\psi(x)$, then $L\psi(x)$ is some new state in the space. L is a *linear operator* if it satisfies the condition

$$L(\alpha\phi_1 + \beta\phi_2) = \alpha(L\phi_1) + \beta(L\phi_2) \qquad ; \text{ linear operator} \tag{2.23}$$

for any (ϕ_1, ϕ_2) in the space. L is *hermitian* if it satisfies the relation[4]

$$\int dx\, \phi_1^\star(x) L\phi_2(x) = \int dx\, [L\phi_1(x)]^\star \phi_2(x) = \left[\int dx\, \phi_2^\star(x) L\phi_1(x)\right]^\star \qquad ; \text{ hermitian} \tag{2.24}$$

A shorthand for these relations is as follows

$$\langle\phi_1|L|\phi_2\rangle = \langle L\phi_1|\phi_2\rangle = \langle\phi_2|L|\phi_1\rangle^\star \qquad ; \text{ shorthand} \tag{2.25}$$

We now make the important observation that *if one knows the matrix elements of* L

$$L_{mn} \equiv \int dx\, \phi_m^\star(x) L\phi_n(x) \equiv \langle m|L|n\rangle \qquad ; \text{ matrix elements} \tag{2.26}$$

in any complete basis, then one knows the operator L. Let us prove this assertion. Let $\psi(x)$ be an arbitrary state in the space. If one knows the corresponding $L\psi(x)$, then L is determined. Expand $\psi(x)$ in the complete basis

$$\psi(x) = \sum_n c_n \phi_n(x) \qquad ; \text{ complete basis} \tag{2.27}$$

As above, the coefficients c_n follow from the orthonormality of the eigenfunctions ϕ_n

$$c_n = \int dx\, \phi_n^\star(x)\psi(x) \qquad ; \text{ known} \tag{2.28}$$

These coefficients are thus determined for any given ψ. Now compute[5]

$$L\psi(x) = \sum_n c_n [L\phi_n(x)] \tag{2.29}$$

[4] See ProbI. 4.5—the notation "ProbI" refers to the problems in Vol. I.

[5] It is assumed here that there is enough convergence that one can operate on this series term by term.

The expansion in a complete basis can again be invoked to write the state $L\phi_n(x)$ as

$$L\phi_n(x) = \sum_m \beta_{mn}\phi_m(x) \qquad ; \text{ complete basis} \tag{2.30}$$

and the orthonormality of the eigenfunctions allows one to identify

$$\beta_{mn} = \int dx\, \phi_m^\star(x) L\phi_n(x) = L_{mn} \tag{2.31}$$

Hence

$$\begin{aligned} L\phi_n(x) &= \sum_m \phi_m(x) L_{mn} \\ \Rightarrow \qquad L\psi(x) &= \sum_n \sum_m \phi_m(x) L_{mn} c_n \qquad ; \text{ known} \end{aligned} \tag{2.32}$$

This is now a *known quantity*, and thus we have established the equivalence[6]

$$L \longleftrightarrow L_{mn} \qquad ; \text{ equivalent} \tag{2.33}$$

2.3.1 *Eigenfunctions*

The *eigenfunctions* of a linear operator are defined by the relation

$$\begin{aligned} L\phi_\lambda(x) = \lambda\phi_\lambda(x) \qquad &; \text{ eigenfunctions} \\ &\lambda \text{ is eigenvalue} \end{aligned} \tag{2.34}$$

Here the operator simply reproduces the function and multiplies it by a constant, the *eigenvalue*. If L is an *hermitian* operator, then the following results hold:

- The eigenvalues λ are real (ProbI. 4.6);
- The eigenfunctions corresponding to different eigenvalues are orthogonal.[7]

We give two examples from Vol. I:

(1) *Momentum.* The momentum operator in one dimension in coordinate space is

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad ; \text{ momentum} \tag{2.35}$$

[6]This equivalence is the basis of *matrix mechanics* (compare Prob. 2.8).
[7]The proof here is essentially that of ProbI. H.4; dedicated readers can supply it.

With periodic boundary conditions, the eigenfunctions are just those of Eq. (2.9), and

$$p\phi_k(x) = \hbar k\, \phi_k(x) \qquad ;\ k = \frac{2\pi n}{L} \qquad ;\ n = 0, \pm 1, \cdots \tag{2.36}$$

p is hermitian with these boundary conditions (ProbI. 4.5), and as we have seen, these eigenfunctions are both orthonormal and complete.

(2) *Hamiltonian.* In one dimension in coordinate space the hamiltonian is given by

$$H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \qquad ;\ \text{hamiltonian} \tag{2.37}$$

We assume that $V(x)$ is real. The eigenstates are

$$Hu_{E_n}(x) = E_n\, u_{E_n}(x) \qquad ;\ \text{eigenstates} \tag{2.38}$$

In general, there will be both bound-state and continuum solutions to this equation. With the choice of periodic boundary conditions in the continuum, the hamiltonian is hermitian (ProbI. 4.5), and the energy eigenvalues E_n are real (ProbI. 4.6). The eigenstates of this hermitian operator also form a *complete set*, so that one can similarly expand an arbitrary $\psi(x)$ as

$$\psi(x) = \sum_n a_n\, u_{E_n}(x) \qquad ;\ \text{complete set} \tag{2.39}$$

For the present purposes, one can simply take two of the postulates of quantum mechanics to be:

(1) Observables are represented with linear hermitian operators;
(2) The eigenfunctions of any linear hermitian operator form a complete set.[8]

2.3.2 *Eigenstates of Position*

The position operator x in one dimension is an hermitian operator. Consider the eigenstates of x with eigenvalues ξ so that

$$x\psi_\xi(x) = \xi\, \psi_\xi(x) \qquad ;\ \text{position operator} \tag{2.40}$$

[8] A proof of completeness for any operator of the Sturm-Liouville type is contained in [Fetter and Walecka (2003)]. The use of ordinary riemannian integration in the definition of the inner product in Eq. (2.19), and the notion of completeness expressed in Eq. (2.14), represent the extent of the mathematical rigor in the present discussion.

The solution to this equation, in coordinate space, is just a Dirac delta function

$$\psi_\xi(x) = \delta(x-\xi) \qquad ;\ \text{eigenstates of position} \tag{2.41}$$

It is readily verified that

$$x\psi_\xi(x) = x\delta(x-\xi) = \xi\delta(x-\xi) = \xi\,\psi_\xi(x) \tag{2.42}$$

On the interval $[0, L]$, with periodic boundary conditions, the eigenvalues ξ run continuously over this interval. As to the orthonormality of these eigenfunctions, one can just compute

$$\int dx\,\psi^\star_{\xi'}(x)\psi_\xi(x) = \int dx\,\delta(x-\xi')\delta(x-\xi) = \delta(\xi-\xi') \tag{2.43}$$

Hence

$$\int dx\,\psi^\star_{\xi'}(x)\psi_\xi(x) = \delta(\xi-\xi') \qquad ;\ \text{orthonormality} \tag{2.44}$$

We make some comments on this result:

- One cannot avoid a continuum normalization here, since the position eigenvalue ξ is truly continuous;
- In contrast, in one dimension with periodic boundary conditions on this interval, the eigenfunctions of momentum in Eq. (2.36) have a *denumerably infinite set of discrete eigenvalues*. This proved to be an essential calculational tool in Vol. I;
- To make the analogy between coordinate space and momentum space closer, one can take L to infinity.[9] Define

$$\psi_k(x) = \left(\frac{L}{2\pi}\right)^{1/2}\phi_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx} \tag{2.45}$$

Then

$$\begin{aligned}\int dx\,\psi^\star_{k'}(x)\psi_k(x) \;&=\; \frac{1}{2\pi}\int dx\,e^{i(k-k')x} \\ &\to \delta(k-k') \qquad\qquad ;\ L\to\infty\end{aligned} \tag{2.46}$$

In this limit *both* the momentum and position eigenfunctions have a continuum norm.

[9] As shown in Vol. I, Fourier series are converted to Fourier integrals in this limit; one first uses the p.b.c. to convert the interval to $[-L/2, L/2]$.

2.4 Abstract Hilbert Space

Recall Eqs. (2.12) and (2.20) from above, which represent an expansion in a complete set,

$$\psi(x) = \sum_n c_n \phi_n(x)$$
$$\text{or ;} \qquad \psi_x = \sum_n c_n [\phi_n]_x \tag{2.47}$$

This can be viewed as the component form of the abstract vector relation

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle \qquad \text{; abstract vector relation} \tag{2.48}$$

Just as an ordinary three-dimensional vector $\mathbf{v}$ has meaning independent of the basis vectors in which it is being decomposed, one can think of this as a vector pointing in some direction in the abstract, infinite-dimensional Hilbert space. Equations (2.47) then provide a component form of this abstract vector relation.

2.4.1 *Inner Product*

The inner product in this space is provided by Eq. (2.19)

$$\langle \psi_a | \psi_b \rangle = \sum_x [\psi_a]_x^\star [\psi_b]_x \equiv \int dx\, \psi_a^\star(x) \psi_b(x) \qquad \text{; inner product} \tag{2.49}$$

Thus, from Eqs. (2.47)

$$c_n = \langle \phi_n | \psi \rangle = \sum_x [\phi_n]_x^\star \psi_x \equiv \int dx\, \phi_n^\star(x) \psi(x) \tag{2.50}$$

We note the following important inner products:

$$\langle \xi' | \xi \rangle = \int dx\, \psi_{\xi'}^\star(x) \psi_\xi(x) = \delta(\xi' - \xi)$$
$$\langle k' | k \rangle = \int dx\, \phi_{k'}^\star(x) \phi_k(x) = \delta_{kk'} \qquad \text{; with p.b.c.}$$
$$\langle \xi | k \rangle = \int dx\, \psi_\xi^\star(x) \phi_k(x) = \frac{1}{\sqrt{L}} e^{ik\xi} \tag{2.51}$$

The last relation follows directly from the wave functions in Eqs. (2.36) and (2.41).[10]

[10] See also Eq. (2.9); note that the subscript n on $k_n = 2\pi n/L$ is suppressed.

2.4.2 *Completeness*

As established in Vol. I, the statement of completeness with the set of coordinate space eigenfunctions $\phi_p(x)$, where p denotes the eigenvalues of a linear hermitian operator, is

$$\sum_p \phi_p(x)\phi_p^\star(y) = \delta(x-y) \qquad ;\text{ completeness} \tag{2.52}$$

Insert this relation in the definition of the inner product in Eq. (2.49)

$$\begin{aligned}\langle\psi_a|\psi_b\rangle &= \int dx\,\psi_a^\star(x)\psi_b(x) \equiv \int dxdy\,\psi_a^\star(x)\delta(x-y)\psi_b(y)\\ &= \sum_p \int dx\,\psi_a^\star(x)\phi_p(x)\int dy\,\phi_p^\star(y)\psi_b(y)\\ &= \sum_p \langle\psi_a|\phi_p\rangle\langle\phi_p|\psi_b\rangle\end{aligned} \tag{2.53}$$

Here Eq. (2.52) has been used in the second line, and the definition of the inner product used in the third. This relation can be summarized by writing the abstract vector relation

$$\sum_p |\phi_p\rangle\langle\phi_p| = 1_{\rm op} \qquad ;\text{ completeness} \tag{2.54}$$

This unit operator $1_{\rm op}$ can be inserted into any inner product, leaving that inner product unchanged. This relation follows from the completeness of the wave functions $\phi_p(x)$ providing the coordinate space components of the abstract state vectors $|\phi_p\rangle$.

2.4.3 *Linear Hermitian Operators*

In Vol. I, quantum mechanics was introduced in coordinate space, where the momentum p is given by $p = (\hbar/i)\partial/\partial x$. It was observed in ProbI. 4.8 that one could equally well work in momentum space, where the position x is given by $x = i\hbar\partial/\partial p$. It was also observed there that the commutation relation $[p, x] = \hbar/i$ is independent of the particular representation. Our goal in this section is to similarly *abstract the Schrödinger equation* and free it from any particular component representation.

2.4.3.1 *Eigenstates*

A linear hermitian operator $L_{\rm op}$ takes one abstract vector $|\psi\rangle$ into another $L_{\rm op}|\psi\rangle$. The eigenstates of $L_{\rm op}$, as before, are defined by

$$L_{\rm op}|\phi_\lambda\rangle = \lambda|\phi_\lambda\rangle \qquad ;\ \text{eigenstates} \tag{2.55}$$

For example:

$$\begin{aligned} p_{\rm op}|k\rangle &= \hbar k|k\rangle && ;\ \text{momentum} \\ x_{\rm op}|\xi\rangle &= \xi|\xi\rangle && ;\ \text{position} \\ (L_z)_{\rm op}|m\rangle &= m|m\rangle && ;\ \text{z-component of angular momentum} \\ H_{\rm op}|\psi\rangle &= E|\psi\rangle && ;\ \text{hamiltonian} \end{aligned} \tag{2.56}$$

2.4.3.2 *Adjoint Operators*

In coordinate space, the adjoint operator $L^\dagger$ is defined by

$$\int d\xi\, \psi_a^\star(\xi) L^\dagger \psi_b(\xi) \equiv \int d\xi\, [L\psi_a(\xi)]^\star \psi_b(\xi) = \left[\int d\xi\, \psi_b^\star(\xi) L\psi_a(\xi)\right]^\star \tag{2.57}$$

The adjoint operator in the abstract Hilbert space is defined in exactly the same manner

$$\langle\psi_a|L_{\rm op}^\dagger|\psi_b\rangle \equiv \langle L_{\rm op}\psi_a|\psi_b\rangle = \langle\psi_b|L_{\rm op}|\psi_a\rangle^\star \qquad ;\ \text{adjoint} \tag{2.58}$$

Note that it follows from this definition that if γ is some complex number, then

$$[\gamma L_{\rm op}]^\dagger = \gamma^\star L_{\rm op}^\dagger \tag{2.59}$$

An operator is *hermitian* if it is equal to its adjoint

$$\begin{aligned} & L_{\rm op}^\dagger = L_{\rm op} && ;\ \text{hermitian} \\ \Rightarrow \quad & \langle\psi_a|L_{\rm op}|\psi_b\rangle = \langle L_{\rm op}\psi_a|\psi_b\rangle = \langle\psi_b|L_{\rm op}|\psi_a\rangle^\star \end{aligned} \tag{2.60}$$

With an hermitian operator, one can just let it act on the state on the left when calculating matrix elements.

2.4.4 *Schrödinger Equation*

To get the time-independent Schrödinger equation in the coordinate representation, one projects the abstract operator relation $H_{\rm op}|\psi\rangle = E|\psi\rangle$ onto the basis of eigenstates of position $|\xi\rangle$.

We show this through the following set of steps:

(1) First project $|\psi\rangle$ onto an eigenstate of position $|\xi\rangle$

$$\langle\xi|\psi\rangle = \sum_x [\psi_\xi]^\star_x [\psi]_x = \int dx\, \psi^\star_\xi(x)\psi(x) = \int dx\, \delta(\xi - x)\psi(x)$$
$$\langle\xi|\psi\rangle = \psi(\xi) \qquad ;\ \text{wave function} \tag{2.61}$$

This is simply the familiar coordinate space wave function $\psi(\xi)$;

(2) Compute the matrix element of the potential $V_{\rm op} = V(x_{\rm op})$ between eigenstates of position

$$\langle\xi|V_{\rm op}|\xi'\rangle = \langle\xi|V(x_{\rm op})|\xi'\rangle = V(\xi')\langle\xi|\xi'\rangle = V(\xi)\delta(\xi - \xi') \tag{2.62}$$

(3) Similarly, compute the matrix elements of the kinetic energy $T_{\rm op}$. This is readily accomplished by invoking the completeness relation for the eigenstates of momentum [see Eq. (2.54)]

$$\sum_k |k\rangle\langle k| = 1_{\rm op} \qquad ;\ \text{completeness} \tag{2.63}$$

With the insertion of this relation (twice), one finds

$$\begin{aligned}\langle\xi|T_{\rm op}|\xi'\rangle &= \frac{1}{2m}\langle\xi|p^2_{\rm op}|\xi'\rangle = \frac{1}{2m}\sum_k\sum_{k'}\langle\xi|k\rangle\langle k|p^2_{\rm op}|k'\rangle\langle k'|\xi'\rangle \\ &= \frac{\hbar^2}{2m}\sum_k\sum_{k'}\langle\xi|k\rangle k^2\delta_{kk'}\langle k'|\xi'\rangle = \frac{\hbar^2}{2m}\sum_k \frac{k^2}{L}e^{ik(\xi-\xi')} \\ &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2}\sum_k \frac{1}{L}e^{ik(\xi-\xi')} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2}\delta(\xi - \xi')\end{aligned} \tag{2.64}$$

The final relation follows from the completeness of the momentum wave functions.

(4) Make use of the statement of completeness of the abstract eigenstates of position, which is

$$\int d\xi\, |\xi\rangle\langle\xi| = 1_{\rm op} \qquad ;\ \text{completeness} \tag{2.65}$$

Note that the sum here is actually an integral because the position eigenvalues are continuous.[11]

[11] See Prob. 2.2.

(5) The operator form of the time-independent Schrödinger equation is

$$H_{\rm op}|\psi\rangle = (T_{\rm op} + V_{\rm op})|\psi\rangle = E|\psi\rangle \qquad ;\ \text{S-equation} \tag{2.66}$$

A projection of this equation on the eigenstates of position gives

$$\langle\xi|H_{\rm op}|\psi\rangle = E\langle\xi|\psi\rangle = E\psi(\xi) \tag{2.67}$$

Now insert Eq. (2.65) in the expression on the l.h.s., and use the results from Eqs. (2.62) and (2.64)

$$\begin{aligned}\langle\xi|H_{\rm op}|\psi\rangle &= \int d\xi'\,\langle\xi|H_{\rm op}|\xi'\rangle\langle\xi'|\psi\rangle \\ &= \int d\xi'\,\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2} + V(\xi)\right]\delta(\xi-\xi')\psi(\xi') \\ &= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2} + V(\xi)\right]\int d\xi'\,\delta(\xi-\xi')\psi(\xi') \\ &= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2} + V(\xi)\right]\psi(\xi)\end{aligned} \tag{2.68}$$

Thus, in summary,

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2} + V(\xi)\right]\psi(\xi) = E\,\psi(\xi) \qquad ;\ \text{S-equation} \tag{2.69}$$

This is just the time-independent Schrödinger equation in the coordinate representation. It is the component form of the operator relation of Eq. (2.66) in a basis of eigenstates of position.[12]

For the *time-dependent Schrödinger equation*, the state vector $|\Psi(t)\rangle$ simply moves in the abstract Hilbert space with a time dependence generated by the hamiltonian. Quantum dynamics is thus summarized in the following relations

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle &= \hat{H}|\Psi(t)\rangle \qquad &;\ \text{S-equation} \\ [\hat{p},\hat{x}] &= \frac{\hbar}{i} \qquad &;\ \text{C.C.R.}\end{aligned} \tag{2.70}$$

We make several comments:

[12]The time-independent Schrödinger equation in the momentum representation is obtained by projecting Eq. (2.66) onto the states $|k\rangle$. This gives the components of the operator relation in a basis of eigenstates of momentum (see Prob. 2.9).

- Here, and henceforth, we shall use a caret over a symbol to denote an operator in the abstract Hilbert space;[13]
- The first equation is the abstract form of the time-dependent Schrödinger equation;
- The second equation is the canonical commutation relation for the momentum and position operators;
- As shown above, the usual Schrödinger equation in coordinate space is obtained by projecting the first relation on eigenstates of position; however, these relations are now *independent of the particular basis in which we choose to express their components.*

2.4.4.1 *Stationary States*

With a time-independent potential, one can again look for normal-mode solutions to the time-dependent Schrödinger Eq. (2.70) of the form

$$|\Psi(t)\rangle = e^{-iEt/\hbar}|\psi\rangle \qquad ; \text{ normal modes} \tag{2.71}$$

Substitution into the first of Eqs. (2.70), and cancellation of a factor $\exp(-iEt/\hbar)$, leads to the stationary-state Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle \qquad ; \text{ stationary-state S-eqn} \tag{2.72}$$

2.5 Measurements

We must establish the relation between these formal developments and physical measurements. Measurement theory is a deep and extensive topic, and we certainly shall not do justice to it here. No attempt is made to consider implications for very complex objects with a myriad of degrees of freedom.[14] Rather, the discussion here focuses on simple systems where measurement theory is really quite intuitive.

2.5.1 *Coordinate Space*

We start in coordinate space and abstract later. An observable F is represented by a linear hermitian operator (H, p, x, L_z, *etc.*) with an (assumed)

[13] Except for the creation and destruction operators, where their operator nature is evident (see later).

[14] Schrödinger's cat, for example (see [Wikipedia (2009)]).

complete set of eigenstates[15]

$$F u_{f_n}(x) = f_n\, u_{f_n}(x) \qquad ;\ \text{eigenstates}$$
$$\text{eigenvalues } f_1, f_2, \cdots, f_\infty \tag{2.73}$$

Let $\Psi(x,t)$ be an arbitrary wave function. At a given time t, its spatial dependence can be expanded in the complete set of wave functions $u_{f_n}(x)$

$$\Psi(x,t) = \sum_n a_{f_n}(t)\; u_{f_n}(x) \tag{2.74}$$

The wave function is assumed to be normalized so that

$$\int dx\, |\Psi(x,t)|^2 = \sum_n |a_{f_n}(t)|^2 = 1 \tag{2.75}$$

We can *measure* the expectation value of F given by[16]

$$\langle F\rangle = \int dx\, \Psi^\star(x,t) F \Psi(x,t) = \sum_n \sum_{n'} a^\star_{f_n}(t) a_{f_{n'}}(t) \int dx\, u^\star_{f_n}(x) F u_{f_{n'}}(x)$$
$$= \sum_n \sum_{n'} a^\star_{f_n}(t) a_{f_{n'}}(t) f_n \delta_{nn'} \tag{2.76}$$

Hence

$$\langle F\rangle = \sum_n |a_{f_n}(t)|^2 f_n \qquad ;\ \text{expectation value} \tag{2.77}$$

If one is in a stationary state so that

$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar} \qquad ;\ \text{stationary state} \tag{2.78}$$

then the wave function $\psi(x)$ can be expanded in the $u_{f_n}(x)$ with time-independent coefficients a_{f_n}

$$\psi(x) = \sum_n a_{f_n}\, u_{f_n}(x) \qquad ;\ \text{completeness} \tag{2.79}$$

It follows as above that in this case

$$1 = \sum_n |a_{f_n}|^2$$
$$\langle F\rangle = \sum_n |a_{f_n}|^2 f_n \qquad ;\ \text{stationary state} \tag{2.80}$$

[15] For clarity, we present the following arguments in one dimension.
[16] See ProbI. 4.5.

If one is also in an eigenstate of F, then

$$\langle F\rangle = f_n \qquad ;\text{ in eigenstate} \tag{2.81}$$

Equations (2.77) and (2.75) suggest that one should interpret the quantity $|a_{f_n}(t)|^2$ as the *probability of measuring the value f_n at the time t if a system is in the state $\Psi(x,t)$*. Based on this argument, we make the following *measurement postulates*:

(1) If one makes a precise measurement of F, then one *must observe one of the eigenvalues f_n*;
(2) If one is in an arbitrary state $\Psi(x,t)$, then $|a_{f_n}(t)|^2$ is the probability that one will observe the value f_n for F at the time t, where[17]

$$a_{f_n}(t) = \int dx\, u^\star_{f_n}(x)\Psi(x,t) \tag{2.82}$$

As an example, consider the free-particle wave packet of Vol. I

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\, A(k)e^{i(kx-\omega_k t)} \qquad ;\text{ free particle} \tag{2.83}$$

The probability density in coordinate space is $|\Psi(x,t)|^2$. The Fourier transform of this relation gives

$$\frac{1}{\sqrt{2\pi}}\int dx\, e^{-ikx}\Psi(x,t) = A(k)e^{-i\omega_k t} \tag{2.84}$$

For localized wave packets, one can take $u_p(x) = e^{ikx}/\sqrt{2\pi}$ as the eigenstates of momentum. Then, consistent with our interpretation in Vol. I,

$$|A(k)|^2 = \left|\int dx\, u^\star_p(x)\Psi(x,t)\right|^2 \qquad ;\ p = \hbar k \tag{2.85}$$

is the *probability density in momentum space* (see ProbI. 4.8).

2.5.2 *Abstract Form*

One can now proceed to *abstract* these results:

(1) The quantity F is represented with a linear hermitian operator $\hat{F}$ with eigenstates

$$\hat{F}|f_n\rangle = f_n|f_n\rangle \tag{2.86}$$

[17] Alternatively, if one has a large number of identical systems with wave function $\Psi(x,t)$, then the fraction of measurements yielding f_n will be $|a_{f_n}(t)|^2$.

If one makes a precise measurement of F, then one will observe one of the eigenvalues f_n.

(2) An arbitrary state $|\Psi(t)\rangle$ can be expanded in the (assumed) complete set of eigenstates of $\hat{F}$ according to

$$|\Psi(t)\rangle = \sum_n a_{f_n}(t)|f_n\rangle \tag{2.87}$$

Then the probability that a measurement will yield the value f_n is

$$|a_{f_n}(t)|^2 = |\langle f_n|\Psi(t)\rangle|^2 \tag{2.88}$$

In particular, $|\langle\xi|\Psi(t)\rangle|^2 = |\Psi(\xi,t)|^2$ is the *probability density that one will observe the value ξ if one makes a measurement of the position x.* This is how we have used the wave function $\Psi(\xi,t)$. Now everything stands on the same footing, and the above contains all our previous assumptions concerning the physical interpretation of the theory.

2.5.3 *Reduction of the Wave Packet*

If a particle moves in a classical orbit, its position can be measured and one finds a value q. If the measurement is repeated a short time Δt later, such that $|\Delta q| \ll |q|$, one must again find the value q. *Measurements must be reproducible.* How does this show up in quantum mechanics?

If one measures the quantity F at the time t and finds a value f_n, then if F is measured again right away, must again find the value f_n. *This is an assumption of the reproducibility of measurements.*

Suppose one is in the state

$$\Psi(x,t) = \sum_n a_{f_n}(t)u_{f_n}(x) \tag{2.89}$$

If one measures F at the time t_0 and finds a value f_n, then right after this measurement, the wave function must be such as *to again give the value* f_n, and it must be normalized. Thus, with no degeneracy, the effect of this measurement is to *reduce* the wave function to the form[18]

$$\Psi(x,t_0)' = \frac{a_{f_n}(t_0)}{|a_{f_n}(t_0)|}u_{f_n}(x) \tag{2.90}$$

This result can be abstracted and extended to lead to an additional measurement postulate:

[18]We speak here of "pure pass measurements" that do not modify the coefficients $a_{f_n}(t)$.

(3) If, at the time t_0, one observes a value f for the quantity F which lies in the inteval $f' \leq f \leq f''$, then the state vector is reduced to

$$|\Psi(t_0)\rangle' = \frac{\sum'_n a_{f_n}(t_0)|f_n\rangle}{\left(\sum'_n |a_{f_n}(t_0)|^2\right)^{1/2}} \quad ; \text{ where } f' \leq f_n \leq f'' \tag{2.91}$$

Here $\sum'_n$ implies $f' \leq f_n \leq f''$.

Although this postulate may at first seem very mysterious, a little reflection will convince the reader that a measurement does indeed provide a great deal of information about a system, in particular, this type of information. We briefly discuss, as an example, the classic Stern-Gerlach experiment.

2.5.4 *Stern-Gerlach Experiment*

The first moral here is that in applying measurement theory, one must always discuss the specific measurement in detail.[19] Consider, for illustration, a spinless, positively-charged particle in a metastable p-state in a neutral atom, where there is no Lorentz force on the atom. There are three possible values of L_z, the angular momentum in the z-direction, $m = 0, \pm 1$. This atom has a magnetic moment, and if placed in a magnetic field which determines the z-direction, and which also *varies* in the z-direction, it will feel a force in the z-direction of

$$F_z = \mu_z \frac{dB_z}{dz} \tag{2.92}$$

This force acts differently on the different m components, and can be used to separate them. Suppose a beam of these atoms, produced, say, in an oven, is passed through an appropriate inhomogeneous magnet as sketched in Fig. 2.1. We then note the following:

- The beam will subsequently *split into three separate components with* $m = 0, \pm 1$. Each beam can be caused to pass through a separate slit as shown in Fig. 2.1. *This illustrates that one observes the eigenvalues of* L_z.
- Initially, the internal wave function of an atom can be written

$$\psi_{\text{int}}(\mathbf{x}, t) = R_{np}(r) \sum_{m=0,\pm 1} c_m(t) Y_{1m}(\theta, \phi) \tag{2.93}$$

[19] See chapter IV of [Gottfried (1966)] for a thorough discussion of the measurement process.

If the center-of-mass of the atom goes through the top slit (this will happen with probability $|c_{+1}(t_0)|^2$ where t_0 is the time it goes through the magnet), then the *internal* wave function of the atom must be[20]

$$\psi_{\text{int}}(\mathbf{x},t) = \frac{c_{+1}(t_0)}{|c_{+1}(t_0)|} R_{np}(r) Y_{11}(\theta,\phi) e^{-iE_{np}(t-t_0)/\hbar} \qquad (2.94)$$

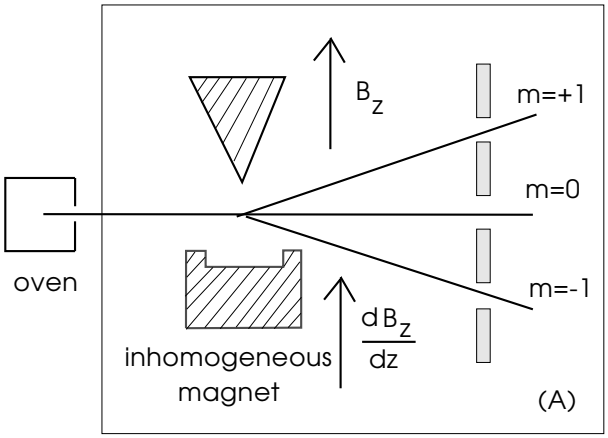

Fig. 2.1 Sketch of the Stern-Gerlach experiment. We will refer to the entire boxed unit as detector (A).

If a second detector identical to (A) in Fig. 2.1 is placed after the top slit, the beam will be observed to pass through and emerge from *its* top slit with unit probability (see Fig. 2.2). *This illustrates the reproduciblity of the measurement.*

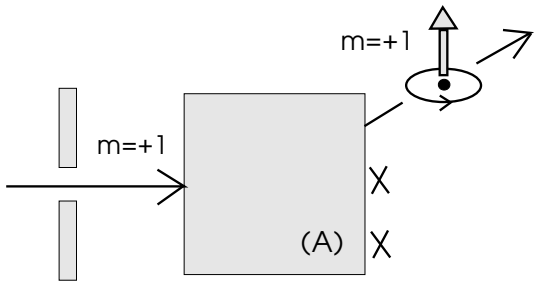

Fig. 2.2 Detector (A) placed after the upper beam with $m = +1$ in Fig. 2.1.

[20] Again, we assume a "pure pass measurement" here.

- If one looks for a beam emerging from the middle and bottom slits of the second detector, there will be none. *This illustrates the reduction of the wave packet by the first measurement.*

Whenever you run into apparent paradoxes in discussing the measurement process, you should always return to this simple and fundamental example of the analysis.

2.6 Quantum Mechanics Postulates

Here we *summarize* the quantum mechanics postulates arrived at in the previous discussion. They are formulated in the abstract Hilbert space.

(1) There is a state vector $|\Psi(t)\rangle$ that provides a complete dynamical description of a system;
(2) An observable F is represented by a linear hermitian operator $\hat{F}$;
(3) The operators obey canonical commutation relations, in particular

$$[\hat{p}, \hat{x}] = \frac{\hbar}{i} \tag{2.95}$$

(4) The dynamics is given by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \tag{2.96}$$

(5) The eigenstates of a linear hermitian operator form a complete set

$$\hat{F}|f_n\rangle = f_n |f_n\rangle \qquad ; \sum_n |f_n\rangle\langle f_n| = \hat{1} \tag{2.97}$$

(6) Measurement postulate:
   (a) A precise measurement of F must yield one of the eigenvalues f_n;
   (b) The probability of observing an eigenvalue f_n at the time t is $|\langle f_n|\Psi(t)\rangle|^2$;
   (c) A measurement $f' \leq f \leq f''$ at time t_0 reduces the state vector to

$$|\Psi(t_0)\rangle' = \frac{\sum'_n a_{f_n}(t_0)|f_n\rangle}{\left(\sum'_n |a_{f_n}(t_0)|^2\right)^{1/2}} \qquad ; \text{ where } f' \leq f_n \leq f'' \tag{2.98}$$

Through his many years in physics, the author has found this to be a complete and essential set of postulates for the implementation of quantum mechanics.

2.7 Many-Particle Hilbert Space

The previous discussion has effectively focused on the quantum mechanics of a single particle. Most of the applications discussed in Vol. I involve many-body systems: atoms, nuclei, hadrons, and quantum fluids. The goal of this section is to extend the previous analysis to the *abstract many-particle Hilbert space*, and to make a connection with quantum field theory as presented in chapter 12 of Vol. I. We start with a summary of the one-dimensional simple harmonic oscillator in abstract Hilbert space.

2.7.1 *Simple Harmonic Oscillator*

The operator analysis of the one-dimensional simple harmonic oscillator is, in fact, carried out in ProbsI. 4.17–4.18.[21] The creation and destruction operators $(a^\dagger, a)$ are first defined as linear combinations of the momentum and coordinate $(\hat{p}, \hat{q})$. The canonical commutation relations for $(\hat{p}, \hat{q})$ imply that[22]

$$[a, a^\dagger] = 1 \tag{2.99}$$

The hermitian number operator is defined as

$$\begin{aligned} \hat{N} &\equiv a^\dagger a && ;\ \text{number operator} \\ \hat{H} &= \hbar\omega(\hat{N} + 1/2) && ;\ \text{hamiltonian} \end{aligned} \tag{2.100}$$

The second line expresses the hamiltonian in terms of the number operator. As demonstrated in ProbsI. 4.17–4.18, *it follows entirely from the general properties of the linear hermitian operators involved that the spectrum of the number operator consists of the positive integers and zero*

$$\begin{aligned} \hat{N}|n\rangle &= n|n\rangle && ;\ n = 0, 1, 2, \cdots, \infty \\ \hat{N}|0\rangle &= 0 && ;\ \text{ground state} \end{aligned} \tag{2.101}$$

The last relation defines the ground state. It further follows that

$$\begin{aligned} a|n\rangle &= \sqrt{n}\,|n-1\rangle && ;\ \text{destruction operator} \\ a^\dagger|n\rangle &= \sqrt{n+1}\,|n+1\rangle && ;\ \text{creation operator} \end{aligned} \tag{2.102}$$

[21] The reader is again strongly urged to work through those problems (see Prob. 2.1).

[22] We suppress the carets on the creation and destruction operators, since it will henceforth be obvious that they act in the abstract occupation-number Hilbert space.

As shown in ProbI. 4.18, the eigenstates $|n\rangle$ can be explicitly constructed as

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle \tag{2.103}$$

We note that this construction involves a relative phase convention.

The eigenstates of the simple harmonic oscillator in the abstract Hilbert space are both orthonormal and complete

$$\begin{aligned} \langle n|n'\rangle &= \delta_{nn'} \quad ; \text{ orthonormal} \\ \sum_n |n\rangle\langle n| &= \hat{1} \quad ; \text{ complete} \end{aligned} \tag{2.104}$$

2.7.2 *Bosons*

With many identical bosons, one introduces a set of creation and destruction operators satisfying

$$[a_k, a_{k'}^\dagger] = \delta_{kk'} \tag{2.105}$$

Here k denotes a complete set of single-particle quantum numbers appropriate to the problem at hand. The basis vectors in the abstract many-particle Hilbert space are then constructed as the direct product of the basis vectors for each of the single-particle states

$$|n_1 n_2 \cdots n_\infty\rangle \equiv |n_1\rangle|n_2\rangle\cdots|n_\infty\rangle \quad ; \text{ many-body basis states} \tag{2.106}$$

Here the subscripts $\{1, 2, \cdots, \infty\}$ simply represent an ordering of all possible values of k. The effects of the creation and destruction operators for any given mode now follow from the above discussion of the simple harmonic oscillator, and as the operators for the different modes commute, it does not matter where one sits relative to the others.

Quantum fields are then operators in this abstract many-particle Hilbert space. We give three examples from Vol. I:

(1) The normal modes for the transverse oscillations of a continuous string of length L with periodic boundary conditions are given by[23]

$$\phi_k(x) = \frac{1}{\sqrt{L}}e^{ikx} \quad ; \; k = \frac{2\pi m}{L} \quad ; \; m = 0, \pm 1, \pm 2, \cdots \tag{2.107}$$

[23] We again suppress the subscript m on $k_m = 2\pi m/L$.

The string energy, which plays the role of free-field hamiltonian, is then found in terms of the quantum field of the string $\hat{q}(x,t)$, obtained from its classical transverse displacement, and the corresponding quantum momentum density $\hat{\pi}(x,t) = \sigma\partial\hat{q}(x,t)/\partial t$, obtained from its classical transverse motion

$$\hat{q}(x,t) = \sum_k \left(\frac{\hbar}{2\omega_k\sigma L}\right)^{1/2}\left[a_k e^{i(kx-\omega_k t)} + a_k^\dagger e^{-i(kx-\omega_k t)}\right] \;\; ; \; \omega_k = |k|c$$

$$\hat{\pi}(x,t) = \frac{1}{i}\sum_k \left(\frac{\hbar\omega_k\sigma}{2L}\right)^{1/2}\left[a_k e^{i(kx-\omega_k t)} - a_k^\dagger e^{-i(kx-\omega_k t)}\right] \qquad (2.108)$$

Here σ is the mass density, and c is the sound velocity. These operators, which here carry the free-field time dependence, satisfy the canonical equal-time commutation relations

$$[\hat{q}(x,t), \hat{\pi}(x',t')]_{t=t'} = i\hbar\delta(x-x') \qquad (2.109)$$

The free-field hamiltonian is[24]

$$\hat{H} = \frac{\sigma}{2}\int_0^L dx\left\{\left[\frac{\partial\hat{q}(x,t)}{\partial t}\right]^2 + c^2\left[\frac{\partial\hat{q}(x,t)}{\partial x}\right]^2\right\} \qquad (2.110)$$

Substitution of the expressions in Eqs. (2.108) gives

$$\hat{H} = \sum_k \hbar\omega_k(a_k^\dagger a_k + a_k a_k^\dagger) = \sum_k \hbar\omega_k(\hat{N}_k + 1/2) \qquad (2.111)$$

This represents an infinite collection of uncoupled simple harmonic oscillators, as discussed above.
The energy eigenvalues for the whole system are given by[25]

$$\hat{H}|n_1 n_2 \cdots n_\infty\rangle = E_{n_1 n_2 \cdots n_\infty}|n_1 n_2 \cdots n_\infty\rangle$$
$$E_{n_1 n_2 \cdots n_\infty} = \sum_k \hbar\omega_k(n_k + 1/2) \qquad (2.112)$$

The quantity n_k is the number of quanta in the k*th* mode, and in analogy to the quantization of light, we refer to these quanta of the sound waves in a string as *phonons*.

[24]Note $c^2 = \tau/\sigma$ where τ is the tension.

[25]Since the subscripts $\{1, 2, \cdots, \infty\}$ on $(n_1, n_2, \cdots, n_\infty)$ simply label the ordered members of the set $k = (0, \pm 2\pi/L, \pm 4\pi/L, \cdots)$, the second of Eqs. (2.112) can equally well be written as $E_{n_1 n_2 \cdots n_\infty} = \sum_{i=1}^{\infty}\hbar\omega_i(n_i + 1/2)$.

Various interaction terms (non-linearity in the string, a spring attached to the string, *etc.*) can now be written in terms of the fields. Since these interactions do not conserve the number of phonons, they will connect one state to any other in the many-particle Hilbert space.

(2) The quantization of the electromagnetic field in Vol. I follows in an analogous fashion.

(3) The non-relativistic many-body hamiltonian for a collection of identical, massive, spin-zero bosons, each with kinetic energy $T = \mathbf{p}^2/2m = -\hbar^2\boldsymbol{\nabla}^2/2m$, and interacting through an instantaneous two-body potential of the form $V(\mathbf{x}, \mathbf{y})$, can be written as

$$\hat{H} = \int d^3x\, \hat{\psi}^\dagger(\mathbf{x}) T \hat{\psi}(\mathbf{x}) + \frac{1}{2}\int d^3x \int d^3y\, \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y}) V(\mathbf{x},\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}) \tag{2.113}$$

Here the quantum field is defined by

$$\hat{\psi}(\mathbf{x}) \equiv \sum_k a_k\, \phi_k(\mathbf{x}) \tag{2.114}$$

where the $\phi_k(\mathbf{x})$ form a complete set of solutions to a one-body Schrödinger equation appropriate, as a starting basis, for the problem at hand. The fields satisfy the canonical commutation relation

$$[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')] = \delta^{(3)}(\mathbf{x} - \mathbf{x}') \tag{2.115}$$

The time evolution of the many-particle system is now governed by the many-body Schrödinger equation.[26] Here, as in our original formulation of quantum mechanics, the operators in this Schrödinger picture are taken to be time-independent, and all the time dependence derives from the Schrödinger equation. When the number of bosons is a constant of the motion, as in liquid ^{4}He, then this hamiltonian never takes one out of the subspace with given N (See Prob. 2.4).

2.7.3 *Fermions*

In the case of fermions, in order to satisfy the Pauli exclusion principle, one quantizes with *anticommutation* relations instead of commutation relations.

[26] This is called "second quantization", since what were previously single-particle wave functions now become field operators in the abstract many-particle Hilbert space. The formulation of the many-body problem in second quantization is carried out in detail in chapter 1 of [Fetter and Walecka (2003a)].

For a single mode, one then has

$$\{a, a^\dagger\} \equiv aa^\dagger + a^\dagger a = 1$$
$$\{a, a\} = \{a^\dagger, a^\dagger\} = 0 \tag{2.116}$$

The number operator is again defined as

$$\hat{N} \equiv a^\dagger a \qquad ; \text{ number operator} \tag{2.117}$$

It follows that this number operator has eigenvalues 0 and 1 (see Vol. I)

$$\hat{N}|n\rangle = n|n\rangle \qquad ; \; n = 0, 1 \tag{2.118}$$

Furthermore (see ProbI 12.8)

$$a|1\rangle = |0\rangle \qquad ; \; a|0\rangle = 0$$
$$a^\dagger|0\rangle = |1\rangle \qquad ; \; a^\dagger|1\rangle = 0 \tag{2.119}$$

The basis states in the abstract Hilbert space are again formed from the direct product of the single-particle states as in Eq. (2.106); however, since the operators for the different single-particle modes now *anticommute*, one has to keep careful track of the ordering of various terms.

As an example, the non-relativistic many-body hamiltonian for a collection of identical spin-1/2 fermions, each with kinetic energy $T = \mathbf{p}^2/2m = -\hbar^2\boldsymbol{\nabla}^2/2m$, and interacting through an instantaneous two-body spin-independent potential of the form $V(\mathbf{x}, \mathbf{y})$, can again be written as

$$\hat{H} = \int d^3x \, \underline{\hat{\psi}}^\dagger(\mathbf{x}) T \, \underline{\hat{\psi}}(\mathbf{x}) + \frac{1}{2} \int d^3x \int d^3y \, \underline{\hat{\psi}}^\dagger(\mathbf{x}) \underline{\hat{\psi}}^\dagger(\mathbf{y}) V(\mathbf{x}, \mathbf{y}) \, \underline{\hat{\psi}}(\mathbf{y}) \underline{\hat{\psi}}(\mathbf{x}) \tag{2.120}$$

Here the quantum field is defined by

$$\underline{\hat{\psi}}(\mathbf{x}) \equiv \sum_{k\lambda} a_{k\lambda} \, \underline{\phi}_{k\lambda}(\mathbf{x}) \tag{2.121}$$

where the two-component spinors $\underline{\phi}_{k\lambda}(\mathbf{x})$ form a complete set of solutions to a one-body Schrödinger equation again appropriate, as a starting basis, for the problem at hand. The index $\lambda = (\uparrow, \downarrow)$ denotes the two spin projections.[27] The components of the field, in this case, now satisfy the canonical *anticommutation* relation

$$\{\hat{\psi}_\alpha(\mathbf{x}), \hat{\psi}^\dagger_\beta(\mathbf{x}')\} = \delta_{\alpha\beta} \, \delta^{(3)}(\mathbf{x} - \mathbf{x}') \tag{2.122}$$

[27] The spinors with the same coordinate label are to be paired in Eq. (2.120).

Chapter 4

Scattering Theory

Given a hamiltonian $\hat{H}$, the goal of this chapter is to solve the Schrödinger equation for a scattering problem and derive general expressions for the S-matrix, T-matrix, and transition rate, many of whose consequences have already been examined in Vol. I.[1] We work in the abstract Hilbert space.

4.1 Interaction Picture

Assume the hamiltonian can be split into two parts $\hat{H} = \hat{H}_0 + \hat{H}_1$, the first part of which leads to an exactly solvable problem, for example, free quanta with no interactions. $\hat{H}_1$ may, or may not, have an explicit time dependence; that depends on the problem at hand.[2] We then want to solve the Schrödinger equation

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{H}_1 \\ i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle &= \hat{H}\,|\Psi(t)\rangle \qquad ;\ \text{Schrödinger-equation} \end{aligned} \tag{4.1}$$

Define a new state vector $|\Psi_{\rm I}(t)\rangle$ by

$$\begin{aligned} |\Psi_{\rm I}(t)\rangle &\equiv e^{\frac{i}{\hbar}\hat{H}_0 t}|\Psi(t)\rangle \qquad ;\ \text{interaction picture} \\ |\Psi_{\rm I}(0)\rangle &= |\Psi(0)\rangle \qquad ;\ \text{coincide at } t=0 \end{aligned} \tag{4.2}$$

[1] For a comprehensive treatment of scattering theory, see [Goldberger and Watson (2004)].

[2] Scattering in a given external field, for example, may lead to an explicitly time-dependent $\hat{H}_1(t)$.

What equation of motion does this new state satisfy? Just compute

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi_{\rm I}(t)\rangle &= -\hat{H}_0\, e^{\frac{i}{\hbar}\hat{H}_0 t}|\Psi(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t}\, i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle \\ &= -\hat{H}_0\,|\Psi_{\rm I}(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t}(\hat{H}_0+\hat{H}_1)e^{-\frac{i}{\hbar}\hat{H}_0 t}|\Psi_{\rm I}(t)\rangle \end{aligned} \tag{4.3}$$

The terms in $\hat{H}_0$ cancel, and thus

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi_{\rm I}(t)\rangle &= \hat{H}_{\rm I}(t)|\Psi_{\rm I}(t)\rangle \qquad\qquad ;\ \text{interaction picture} \\ \hat{H}_{\rm I}(t) &\equiv e^{\frac{i}{\hbar}\hat{H}_0 t}\,\hat{H}_1\, e^{-\frac{i}{\hbar}\hat{H}_0 t} \end{aligned} \tag{4.4}$$

The advantage of this new formulation is that in the limit $\hat{H}_1 \to 0$, the state $|\Psi_{\rm I}(t)\rangle$ becomes time-independent; the free time variation, which can be extremely rapid, has been explicitly dealt with. Equations (4.2) and (4.4) are said to be a formulation of the problem in the *interaction picture*.

4.2 Adiabatic Approach

We will find that when we try to solve the resulting equations and generate the S-matrix, there will be infinite time integrals to carry out over oscillating integrands. In order to give the theory a well-defined mathematical meaning, we introduce an *adiabatic damping factor* $e^{-\epsilon|t|}$ with $\epsilon \geq 0$, and use the following interaction in the interaction picture

$$\hat{H}^{\epsilon}_{\rm I}(t) \equiv e^{-\epsilon|t|}\hat{H}_{\rm I}(t) \qquad ;\ \text{adiabatic damping} \tag{4.5}$$

> *The theory is then defined to be what is obtained in the limit as* $\epsilon \to 0$.[3]

This is a somewhat archaic approach, and there are more sophisticated ways of doing formal scattering theory, which, however, can easily lead to spurious results if one is not very careful and thoughtful. The great advantage of this adiabatic approach is that it *allows one to do well-defined mathematics at each step.*

One can imagine that the interaction in Eq. (4.5) is being turned on and off very slowly ("adiabatically") as the time $t \to \pm\infty$, that is, in the infinite past and infinite future.[4] This allows us to easily specify the initial and final states in any scattering process, since now as $t \to \pm\infty$,

[3] There may, or may not, be other limits — we will not go there.

[4] Explicitly dealing with the scattering of wave packets can play the same role.

the hamiltonian simply reduces to $\hat{H}_0$, and we know how to solve the non-interacting problem

$$\begin{aligned} \hat{H} &= \hat{H}_0 \qquad\qquad ; \; t \to \pm\infty \\ i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle &= \hat{H}_0\,|\Psi(t)\rangle \\ |\Psi(t)\rangle &= e^{-\frac{i}{\hbar}E_0 t}\,|\psi\rangle \end{aligned} \tag{4.6}$$

Here $|\psi\rangle$ is simply a *solution to the free, time-independent, Schrödinger equation*

$$\hat{H}_0\,|\psi\rangle = E_0|\psi\rangle \tag{4.7}$$

The interaction-picture state vector in Eq. (4.2) is then given in this same limit by

$$\begin{aligned} |\Psi_{\rm I}(t)\rangle &= e^{\frac{i}{\hbar}\hat{H}_0 t}\,|\Psi(t)\rangle = |\psi\rangle \qquad ; \; t \to \pm\infty \\ i\hbar\frac{\partial}{\partial t}|\Psi_{\rm I}(t)\rangle &= 0 \end{aligned} \tag{4.8}$$

Thus, in summary, with the adiabatic approach in the interaction picture, one has

$$\begin{aligned} |\Psi_{\rm I}(t)\rangle &= |\psi\rangle \qquad\qquad ; \; t \to \pm\infty \\ \hat{H}_0\,|\psi\rangle &= E_0|\psi\rangle \end{aligned} \tag{4.9}$$

One starts with an initial state of this type, and then slowly turns on and off the interaction. The transition amplitude into a final state of this type is then calculated. The (transition probability)/(time interval the interaction is on) gives the transition rate,[5] and the path from the transition rate to a cross section was detailed in Vol. I.

It is then necessary to determine what happens when the interaction in Eq. (4.5) is turned on and off adiabatically. This is done through the construction of the *time-development operator* for the problem.

[5]We shall get more sophisticated here and actually derive a general expression for the transition rate itself.

4.3 $\hat{U}$-Operator

Let us look for an operator that develops our system in time

$$\begin{aligned} |\Psi_{\rm I}(t)\rangle &= \hat{U}_\epsilon(t,t_0)|\Psi_{\rm I}(t_0)\rangle \\ i\hbar\frac{\partial}{\partial t}|\Psi_{\rm I}(t)\rangle &= i\hbar\frac{\partial}{\partial t}\hat{U}_\epsilon(t,t_0)|\Psi_{\rm I}(t_0)\rangle = \hat{H}_{\rm I}^\epsilon(t)\hat{U}_\epsilon(t,t_0)|\Psi_{\rm I}(t_0)\rangle \end{aligned} \quad (4.10)$$

If this is to hold for all $|\Psi_{\rm I}(t_0)\rangle$, then $\hat{U}_\epsilon(t,t_0)$ must satisfy the operator relation

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\hat{U}_\epsilon(t,t_0) &= \hat{H}_{\rm I}^\epsilon(t)\hat{U}_\epsilon(t,t_0) \\ \hat{U}_\epsilon(t_0,t_0) &= 1 \end{aligned} \quad (4.11)$$

This differential equation, with its initial condition, can be rewritten as an *integral equation*

$$\hat{U}_\epsilon(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} e^{-\epsilon|t'|}\,\hat{H}_{\rm I}(t')\hat{U}_\epsilon(t',t_0)\,dt' \quad (4.12)$$

It is readily verified that Eqs. (4.11) are reproduced by this expression.

We will try to find a solution to this equation as a power series in $\hat{H}_{\rm I}$.[6] Let us substitute this expression for $\hat{U}_\epsilon(t',t_0)$ in the integrand on the r.h.s.

$$\begin{aligned} \hat{U}_\epsilon(t,t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} e^{-\epsilon|t'|}\,\hat{H}_{\rm I}(t')\,dt' + \\ &\left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} e^{-\epsilon|t'|}\,\hat{H}_{\rm I}(t')\,dt' \int_{t_0}^{t'} e^{-\epsilon|t''|}\,\hat{H}_{\rm I}(t'')\hat{U}_\epsilon(t'',t_0)\,dt'' \end{aligned} \quad (4.13)$$

This expression is still exact. Repeated application of this process leads to the following infinite series in $\hat{H}_{\rm I}$

$$\begin{aligned} \hat{U}_\epsilon(t,t_0) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} e^{-\epsilon|t_1|}\,dt_1 \int_{t_0}^{t_1} e^{-\epsilon|t_2|}\,dt_2 \cdots \int_{t_0}^{t_{n-1}} e^{-\epsilon|t_n|}\,dt_n \times \\ \hat{H}_{\rm I}(t_1)\hat{H}_{\rm I}(t_2)\cdots\hat{H}_{\rm I}(t_n) \end{aligned} \quad (4.14)$$

[6] One can only expect a power series to hold for scattering amplitudes at all energies in the absence of bound states; however, we will eventually "zip things up again" and obtain closed forms that are also valid in the presence of bound states.

By convention, the first term in this series is 1. Note that it is important to keep the *ordering* of the operators $\hat{H}_{\rm I}(t)$ straight in the integrand, since they do not necessarily commute at different times. It is easy to remember the ordering since the operators are *time-ordered*, with the operator at the latest time appearing furthest to the left.

Equation (4.14) can be rewritten in the following manner

$$\hat{U}_\epsilon(t,t_0) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^{t} e^{-\epsilon|t_1|}\, dt_1 \int_{t_0}^{t} e^{-\epsilon|t_2|}\, dt_2 \cdots \int_{t_0}^{t} e^{-\epsilon|t_n|}\, dt_n \times T\left[\hat{H}_{\rm I}(t_1)\hat{H}_{\rm I}(t_2)\cdots\hat{H}_{\rm I}(t_n)\right] \quad ;\ t \geq t_0 \tag{4.15}$$

Here

- All the integrals are now over the full range $\int_{t_0}^{t}$;
- The "T-product" carries the instruction that the operators are to be time-ordered, with the operator at the latest time sitting to the left;
- Each term in the sum is divided by $n!$.

The proof that Eq. (4.15) reproduces Eq. (4.14) is quite simple. There are $n!$ possible orderings of the times in the multiple integral, pick one, say $t_1 > t_2 > t_3 > \cdots > t_n$. All possible time orderings of these integration variables provides a complete enumeration of the region of integration in the multiple integral. The operator in the integrand is time-ordered in each case. But now all of these contributions are *identical* by a change of dummy integration variables. Thus Eq. (4.14) is reproduced.[7]

The *scattering operator* $\hat{S}$ is now defined in the following manner

$$\hat{S} \equiv {\rm Lim}_{\epsilon\to 0}\, {\rm Lim}_{t\to+\infty}\, {\rm Lim}_{t_0\to-\infty}\, \hat{U}_\epsilon(t,t_0) \tag{4.16}$$

One lets the initial time $t_0 \to -\infty$, the final time $t \to +\infty$, and then, at the very end, the limit of the adiabatic damping factor $\epsilon \to 0$ is taken. Thus

$$\begin{aligned}\hat{S} &= {\rm Lim}_{\epsilon\to 0}\, \hat{S}_\epsilon \\ &= {\rm Lim}_{\epsilon\to 0} \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^{\infty} e^{-\epsilon|t_1|}\, dt_1 \cdots \int_{-\infty}^{\infty} e^{-\epsilon|t_n|}\, dt_n \times \\ &\quad T\left[\hat{H}_{\rm I}(t_1)\hat{H}_{\rm I}(t_2)\cdots\hat{H}_{\rm I}(t_n)\right]\end{aligned} \tag{4.17}$$

Everything so far has assumed $t \geq t_0$ in Eqs. (4.11) and the subsequent development; however, one can equally well write these equations for $t \leq t_0$.

[7] The explicit demonstration of this equality for $n = 2$ is assigned as Prob. 4.1.

How is the above analysis modified? Write Eq. (4.12) in the following fashion

$$\hat{U}_\epsilon(t,t_0) = 1 + \frac{i}{\hbar}\int_t^{t_0} e^{-\epsilon|t'|}\,\hat{H}_{\rm I}(t')\hat{U}_\epsilon(t',t_0)\,dt' \tag{4.18}$$

It is readily verified that this expression reproduces Eqs. (4.11), and it is most convenient since the integral now runs in the positive direction if $t_0 \geq t$. A repetition of the above arguments in this case then leads to the following infinite series

$$\hat{U}_\epsilon(t,t_0) = \sum_{n=0}^{\infty}\left(\frac{i}{\hbar}\right)^n \frac{1}{n!}\int_t^{t_0} e^{-\epsilon|t_1|}\,dt_1 \int_t^{t_0} e^{-\epsilon|t_2|}\,dt_2 \cdots \int_t^{t_0} e^{-\epsilon|t_n|}\,dt_n \times \overline{T}\left[\hat{H}_{\rm I}(t_1)\hat{H}_{\rm I}(t_2)\cdots\hat{H}_{\rm I}(t_n)\right] \quad ;\ t \leq t_0 \tag{4.19}$$

The "$\overline{T}$-product" instructs the operators to be anti-time-ordered such that the operator with the *earliest* time sits to the left. A simple reversal of the limits of integration in each integral then gives the equivalent expression

$$\hat{U}_\epsilon(t,t_0) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \frac{1}{n!}\int_{t_0}^{t} e^{-\epsilon|t_1|}\,dt_1 \int_{t_0}^{t} e^{-\epsilon|t_2|}\,dt_2 \cdots \int_{t_0}^{t} e^{-\epsilon|t_n|}\,dt_n \times \overline{T}\left[\hat{H}_{\rm I}(t_1)\hat{H}_{\rm I}(t_2)\cdots\hat{H}_{\rm I}(t_n)\right] \quad ;\ t \leq t_0 \tag{4.20}$$

We are now in a position to exhibit some of the properties of $\hat{U}_\epsilon(t,t_0)$ from these series expansions:[8]

(1) Since the adjoint of a product is the product of the adjoints in the reverse order, it follows immediately from Eqs. (4.15) and (4.19) that

$$\hat{U}_\epsilon(t,t_0)^\dagger = \hat{U}_\epsilon(t_0,t) \tag{4.21}$$

which holds for both $t > t_0$ and $t < t_0$.

(2) If one ends up back at the start time, no matter whether $t > t_0$ or $t < t_0$, it must be true that

$$\hat{U}_\epsilon(t_0,t)\hat{U}_\epsilon(t,t_0) = 1 \tag{4.22}$$

This follows from the series expansions, and the explicit demonstration of this relation for $n = 2$ is left as Prob. 4.1.

(3) It follows from the results in (1) and (2) that

$$\hat{U}_\epsilon(t,t_0)^\dagger = \hat{U}_\epsilon(t,t_0)^{-1} \quad ;\ \text{unitary} \tag{4.23}$$

[8]Note that relations (1)–(4) hold for finite ϵ.

The time-evolution operator is *unitary*. We know this must be true, since the Schrödinger equation preserves the *norm* of the states. This is now readily verified from the relation

$$\begin{aligned}\langle\Psi_{\rm I}(t)|\Psi_{\rm I}(t)\rangle &= \langle\Psi_{\rm I}(t_0)|\hat{U}_\epsilon(t,t_0)^\dagger\hat{U}_\epsilon(t,t_0)|\Psi_{\rm I}(t_0)\rangle \\ &= \langle\Psi_{\rm I}(t_0)|\hat{U}_\epsilon(t,t_0)^{-1}\hat{U}_\epsilon(t,t_0)|\Psi_{\rm I}(t_0)\rangle \\ &= \langle\Psi_{\rm I}(t_0)|\Psi_{\rm I}(t_0)\rangle \end{aligned} \tag{4.24}$$

(4) If one propagates the system from $t_0 \to t_1$, and then from $t_1 \to t_2$, the result must be the same as propagation from $t_0 \to t_2$. Thus the time-evolution operator must obey the *group property*

$$\hat{U}_\epsilon(t_2,t_1)\hat{U}_\epsilon(t_1,t_0) = \hat{U}_\epsilon(t_2,t_0) \qquad ;\ \text{group property} \tag{4.25}$$

Let us demonstrate this result for $t_2 > t_1 > t_0$. The result in (2) can then be used to extend it to any relative times. For example, if $t_1 > t_2$, just write

$$\begin{aligned}\hat{U}_\epsilon(t_2,t_1)\hat{U}_\epsilon(t_1,t_0) &= \hat{U}_\epsilon(t_2,t_1)\hat{U}_\epsilon(t_1,t_2)\hat{U}_\epsilon(t_2,t_0) \\ &= \hat{U}_\epsilon(t_2,t_0) \qquad ;\ t_1 > t_2 \end{aligned} \tag{4.26}$$

Write out the νth term in the sum on the r.h.s. of Eq. (4.25)

$$\begin{aligned}\hat{U}_\epsilon^{(\nu)}(t_2,t_0) = \left(-\frac{i}{\hbar}\right)^\nu \frac{1}{\nu!}\int_{t_0}^{t_2} e^{-\epsilon|t_1'|}\,dt_1' \cdots \int_{t_0}^{t_2} e^{-\epsilon|t_\nu'|}\,dt_\nu' \times \\ T\left[\hat{H}_{\rm I}(t_1')\hat{H}_{\rm I}(t_2')\cdots\hat{H}_{\rm I}(t_\nu')\right] \end{aligned} \tag{4.27}$$

Now note:

- There are $\nu!/n!m!$ ways to partition the times $t_1' \cdots t_\nu'$ so that n times are greater than the intermediate time t_1, and m times are less than t_1 — pick one;
- Now integrate over all possible relative orderings of the times within this particular partition;
- Then sum over all possible choices of the times within this particular partition. This provides a complete enumeration of the regions of integration for a given (n,m);
- The contributions in the sum are identical by a change of dummy integration variables, giving $\nu!/n!m!$ equal contributions;

- Then sum over all values of (n, m) for which $m + n = \nu$. This provides a complete evaluation of the multiple integral in Eq. (4.27)

$$\hat{U}_\epsilon^{(\nu)}(t_2, t_0) = \frac{1}{\nu!} \sum_{n+m=\nu} \left(-\frac{i}{\hbar}\right)^{n+m} \frac{\nu!}{n!m!} \times \tag{4.28}$$
$$\int_{t_1}^{t_2} e^{-\epsilon|t_1'|}\, dt_1' \cdots \int_{t_1}^{t_2} e^{-\epsilon|t_n'|}\, dt_n'\; T\left[\hat{H}_{\rm I}(t_1') \cdots \hat{H}_{\rm I}(t_n')\right] \times$$
$$\int_{t_0}^{t_1} e^{-\epsilon|t_{n+1}'|}\, dt_{n+1}' \cdots \int_{t_0}^{t_1} e^{-\epsilon|t_{n+m}'|}\, dt_{n+m}'\; T\left[\hat{H}_{\rm I}(t_{n+1}') \cdots \hat{H}_{\rm I}(t_{n+m}')\right]$$

- Finally, use $\sum_\nu \sum_{n+m=\nu} = \sum_n \sum_m$. This establishes Eq. (4.25).

4.4 $\hat{U}$-Operator for Finite Times

We started from the hamiltonian

$$\hat{H}_\epsilon = \hat{H}_0 + e^{-\epsilon|t|}\, \hat{H}_1 \tag{4.29}$$

In the end, we are to take the limit $\epsilon \to 0$, which restores the proper hamiltonian. Let us assume that we have used the preceding analysis to propagate the system from its initial state at $t_0 \to -\infty$ to a finite time such that

$$|t| \ll 1/\epsilon \qquad ;\ \text{finite time} \tag{4.30}$$

Now, for this time,

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \qquad ;\ \text{full } \hat{H} \tag{4.31}$$

In this case, we can write a formal solution to the full Schrödinger equation as[9]

$$|\Psi_i(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t} |\Psi_i(0)\rangle \tag{4.32}$$

Here $|\Psi_i(0)\rangle = |\Psi_{\rm I}^i(0)\rangle$ is the state that has propagated up to the time $t = 0$ from the initial state $|\psi_i\rangle$ prepared at $t_0 \to -\infty$ [see Eqs. (4.2)]. With the aid of the previous time-evolution operator, one can write this state as

$$|\Psi_i(0)\rangle = |\Psi_{\rm I}^i(0)\rangle = \hat{U}_\epsilon(0, -\infty)|\psi_i\rangle \equiv |\psi_i^{(+)}\rangle \tag{4.33}$$

[9]We assume here and henceforth that $\hat{H}_1$ now has no explicit time dependence.

This relation defines $|\psi_i^{(+)}\rangle$. A combination of Eqs. (4.32) and (4.33) allows the solution to the Schrödinger equation at a finite time, which satisfies Eq. (4.30), to be expressed as

$$|\Psi_i(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi_i^{(+)}\rangle \tag{4.34}$$

Some comments:

- This is the full Schrödinger state vector that develops from the state $|\psi_i\rangle$ at $t_0 \to -\infty$;
- One needs the adiabatic damping factor to bring that state vector up to finite time with $|\Psi_i(0)\rangle = \hat{U}_\epsilon(0,-\infty)|\psi_i\rangle \equiv |\psi_i^{(+)}\rangle$;
- From there, one can use the formal solution to the full Schrödinger equation in Eq. (4.34).

We note that under the conditions that one can indeed use the formal solution to the full Schrödinger equation, it follows that the interaction-picture state vector at the time t is given by

$$\begin{aligned}|\Psi_{\rm I}(t)\rangle &= e^{\frac{i}{\hbar}\hat{H}_0 t}|\Psi(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}|\Psi(t_0)\rangle \\ &= e^{\frac{i}{\hbar}\hat{H}_0 t}e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}e^{-\frac{i}{\hbar}\hat{H}_0 t_0}|\Psi_{\rm I}(t_0)\rangle \end{aligned} \tag{4.35}$$

Here $|\Psi_{\rm I}(t_0)\rangle$ is the interaction-picture state vector at the time t_0. But now we can immediately identify the time development operator $\hat{U}(t,t_0)$ from the first of Eqs. (4.10)!

$$\hat{U}(t,t_0) = e^{\frac{i}{\hbar}\hat{H}_0 t}e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}e^{-\frac{i}{\hbar}\hat{H}_0 t_0} \quad ;\ |t|,|t_0| \ll 1/\epsilon \tag{4.36}$$

It is only necessary to keep careful track of the ordering of the operators, and make sure that one never interchanges factors that do not commute.

Several of our previous properties of the time-development operator follow immediately from the expression in Eq. (4.36):

$$\begin{aligned}\hat{U}(t,t_0)^\dagger &= \hat{U}(t_0,t) \\ \hat{U}(t,t_0)^\dagger &= \hat{U}(t,t_0)^{-1} \quad ;\ \text{unitary} \\ \hat{U}(t_1,t_2)\hat{U}(t_2,t_3) &= \hat{U}(t_1,t_3) \quad ;\ \text{group property}\end{aligned} \tag{4.37}$$

4.5 The *S*-Matrix

The interaction-picture state vector in the infinite future $|\Psi_{\rm I}(+\infty)\rangle$ that develops from the interaction-picture state vector in the infinite past

$|\Psi_{\rm I}(-\infty)\rangle$ is obtained with the scattering operator in Eq. (4.17)

$$|\Psi_{\rm I}(+\infty)\rangle = \hat{S}\,|\Psi_{\rm I}(-\infty)\rangle \qquad ;\ \text{scattering operator} \tag{4.38}$$

Now, with the adiabatic damping factor, the interaction state vectors in the infinite past and infinite future are simple, they are just the individual non-interacting state vectors in Eq. (4.9), or linear combinations of them. Thus, if one starts with one such prepared state $|\Psi^i_{\rm I}(-\infty)\rangle = |\psi_i\rangle$, and asks for the probability for finding a particular state $|\psi_f\rangle$ in the final state $|\Psi^i_{\rm I}(+\infty)\rangle$ that evolves, in the presence of all the interactions, from that initial prepared state, one has

$$P_{fi} = |\langle\psi_f|\Psi^i_{\rm I}(+\infty)\rangle|^2 = |\langle\psi_f|\hat{S}\,|\Psi^i_{\rm I}(-\infty)\rangle|^2 = |\langle\psi_f|\hat{S}|\psi_i\rangle|^2 \tag{4.39}$$

This is the probability of finding the initial state $|\psi_i\rangle$ in the final state $|\psi_f\rangle$ *after* the scattering has taken place. Here $|\psi_i\rangle$ and $|\psi_f\rangle$ are eigenstates of the free hamiltonian $\hat{H}_0$. The *amplitude* for this process to take place is given by the S-matrix

$$S_{fi} \equiv \langle\psi_f|\hat{S}|\psi_i\rangle \qquad ;\ S\text{-matrix} \tag{4.40}$$

It was argued in Vol. I that the general form of the S-matrix for a scattering process is

$$S_{fi} = \delta_{fi} - 2\pi i\delta(E_f - E_i)\,\tilde{T}_{fi} \tag{4.41}$$

where $\tilde{T}_{fi}$ is the T-matrix. There will always be an energy-conserving delta function here coming out of any calculation.[10]

The probability of making a *transition* to a state $f \neq i$ is therefore

$$P_{fi} = |2\pi i\delta(E_f - E_i)|^2|\tilde{T}_{fi}|^2 \qquad ;\ \text{probability of transition} \tag{4.42}$$

It was argued in Vol. I that the square of the energy-conserving δ-function is to be interpreted as

$$\begin{aligned} |2\pi i\delta(E_f - E_i)|^2 &= 2\pi\delta(E_f - E_i)\,\frac{1}{\hbar}\int_{-\mathcal{T}/2}^{\mathcal{T}/2} dt\, e^{\frac{i}{\hbar}(E_f - E_i)t} \\ &= \frac{2\pi}{\hbar}\delta(E_f - E_i)\mathcal{T} \qquad ;\ \mathcal{T}\to\infty \end{aligned} \tag{4.43}$$

[10] Compare Eq. (4.53) and Prob. 4.8. In Vol. I we removed some additional factors in the definition of the T-matrix element T_{fi} [see EqI. (7.36) and Eq. (7.38)].

where $\mathcal{T} \to \infty$ is the total time the interaction is turned on. The transition *rate* is then given by

$$\omega_{fi} = \frac{P_{fi}}{\mathcal{T}}$$
$$\omega_{fi} = \frac{2\pi}{\hbar}\delta(E_f - E_i)|\tilde{T}_{fi}|^2 \qquad ;\ \text{transition rate}\ (f \neq i) \tag{4.44}$$

This is the transition rate into *one* final state in the continuum. To get the transition rate into the *group* of states that actually get into our detectors when the states are spaced very close together, one must multiply this expression by the appropriate number of states dn_f. To get a *cross section*, one divides by the incident flux

$$d\sigma = \frac{2\pi}{\hbar}\delta(E_f - E_i)|\tilde{T}_{fi}|^2 \frac{dn_f}{I_{\text{inc}}} \qquad ;\ \text{cross section} \tag{4.45}$$

Some comments:

- All of these expressions were discussed and utilized frequently in Vol. I;
- Eq. (4.44) is the full expression for Fermi's Golden Rule, to all orders in the interaction;
- The derivation of the result for the transition rate involves some refinement when adiabatic switching is invoked, in contrast to the sudden turn-on and turn-off of the interaction in Vol. I; however, a proper derivation of the transition rate in this case, which we shall subsequently carry out, gives essentially the same result

$$S_{fi} = \delta_{fi} - 2\pi i\delta(E_f - E_i)\,\tilde{T}_{fi}$$
$$\omega_{fi} = \frac{2}{\hbar}\delta_{fi}\,\text{Im}\,\tilde{T}_{ii} + \frac{2\pi}{\hbar}\delta(E_f - E_i)|\tilde{T}_{fi}|^2 \quad ;\ \text{transition rate} \tag{4.46}$$

4.6 Time-Independent Analysis

We will now perform some formal manipulations on the above results. Let us try to *explicitly carry out the time integrations* in the general term in the S-matrix in Eq. (4.17), which we rewrite in its initial time-ordered form

$$\langle\psi_f|\hat{S}_\epsilon^{(n)}|\psi_i\rangle = \left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{\infty} e^{-\epsilon|t_1|}\,dt_1 \int_{-\infty}^{t_1} e^{-\epsilon|t_2|}\,dt_2 \cdots \int_{-\infty}^{t_{n-1}} e^{-\epsilon|t_n|}\,dt_n$$
$$\times\langle\psi_f|e^{\frac{i}{\hbar}\hat{H}_0 t_1}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0 t_1} e^{\frac{i}{\hbar}\hat{H}_0 t_2}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0 t_2}\cdots$$
$$\cdots\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0 t_{n-1}} e^{\frac{i}{\hbar}\hat{H}_0 t_n}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0 t_n}|\psi_i\rangle \tag{4.47}$$

Here we have simply written out $\langle\psi_f|\hat{H}_{\rm I}(t_1)\cdots\hat{H}_{\rm I}(t_n)|\psi_i\rangle$ in detail.

We will change variables in the integrals as follows

$$\begin{aligned}
x_1 &= t_1 && ;\ t_1 = x_1 \\
x_2 &= t_2 - t_1 && ;\ t_2 = x_1 + x_2 \\
x_3 &= t_3 - t_2 && ;\ t_3 = x_1 + x_2 + x_3 \\
&\vdots && \vdots \\
x_n &= t_n - t_{n-1} && ;\ t_n = x_1 + x_2 + \cdots + x_n
\end{aligned} \tag{4.48}$$

First, let the hamiltonians $\hat{H}_0$ on either end of the operator in Eq. (4.47) act on $|\psi_i\rangle$ and $|\psi_f\rangle$, which are eigenstates of $\hat{H}_0$ with eigenvalues E_0 and E_f respectively. Equation (4.47) then can be written as

$$\begin{aligned}
\langle\psi_f|\hat{S}^{(n)}_\epsilon|\psi_i\rangle = \left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{\infty} e^{-\epsilon|t_1|}\,dt_1 \int_{-\infty}^{t_1} e^{-\epsilon|t_2|}\,dt_2 \cdots \int_{-\infty}^{t_{n-1}} e^{-\epsilon|t_n|}\,dt_n \\
\times\langle\psi_f|e^{\frac{i}{\hbar}(E_f-E_0)t_1}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0(t_1-t_2)}e^{\frac{i}{\hbar}E_0(t_1-t_2)}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0(t_2-t_3)}e^{\frac{i}{\hbar}E_0(t_2-t_3)}\cdots \\
\cdots e^{-\frac{i}{\hbar}\hat{H}_0(t_{n-1}-t_n)}e^{\frac{i}{\hbar}E_0(t_{n-1}-t_n)}\hat{H}_1|\psi_i\rangle
\end{aligned} \tag{4.49}$$

Next, introduce the change in variables in Eqs. (4.48), starting from the right

$$\begin{aligned}
\langle\psi_f|\hat{S}^{(n)}_\epsilon|\psi_i\rangle = \left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_f-E_0)x_1}e^{-\epsilon|x_1|}\,dx_1 \times \\
\langle\psi_f|\hat{H}_1 \int_{-\infty}^{0} dx_2\, e^{\{-\frac{i}{\hbar}(E_0-\hat{H}_0)x_2-\epsilon|x_1+x_2|\}}\,\hat{H}_1 \times \\
\int_{-\infty}^{0} dx_3\, e^{\{-\frac{i}{\hbar}(E_0-\hat{H}_0)x_3-\epsilon|x_1+x_2+x_3|\}}\,\hat{H}_1 \times \cdots \\
\cdots \hat{H}_1 \int_{-\infty}^{0} dx_n\, e^{\{-\frac{i}{\hbar}(E_0-\hat{H}_0)x_n-\epsilon|x_1+\cdots+x_n|\}}\,\hat{H}_1|\psi_i\rangle
\end{aligned} \tag{4.50}$$

Now *do* all the integrals starting on the right, keeping all the other variables fixed while so doing.

Consider the first integral over dx_n at fixed $(x_1,\cdots,x_{n-1})$. What we really need is $\mathrm{Lim}_{\epsilon\to 0}\,\langle\psi_f|\hat{S}^{(n)}_\epsilon|\psi_i\rangle$. Since the damping factors are just there to cut off the oscillating exponentials, we should get the same results no matter how we go to that limit, if the theory is to make sense. We claim that *in the limit*, we can replace $e^{-\epsilon|x_1+\cdots+x_n|} \doteq e^{\epsilon x_n}$ in the integral over x_n, since it is only important for very large negative x_n. Repetition of this

argument, as we do the integrals from right to left, allows us to replace

$$\begin{aligned}&\text{Lim}_{\,\epsilon\to 0}\int\cdots\int e^{-\epsilon|x_1|}e^{-\epsilon|x_1+x_2|}\cdots e^{-\epsilon|x_1+\cdots x_n|}\cdots=\\&\text{Lim}_{\,\epsilon\to 0}\int\cdots\int e^{-\epsilon|x_1|}e^{\epsilon x_2}\cdots e^{\epsilon x_n}\cdots\end{aligned}\tag{4.51}$$

The integrals now *factor*, and they can all be immediately carried out

$$\begin{aligned}\langle\psi_f|\hat{S}^{(n)}_\epsilon|\psi_i\rangle=\left(-\frac{i}{\hbar}\right)^n 2\pi\hbar\,\delta(E_f-E_0)\times\\ \langle\psi_f|\hat{H}_1\frac{1}{-i(E_0-\hat{H}_0)/\hbar+\epsilon}\hat{H}_1\frac{1}{-i(E_0-\hat{H}_0)/\hbar+\epsilon}\hat{H}_1\cdots\\ \cdots\frac{1}{-i(E_0-\hat{H}_0)/\hbar+\epsilon}\hat{H}_1|\psi_i\rangle\end{aligned}\tag{4.52}$$

The operator $\hat{H}_1$ appears n times in this expression. This equation has meaning in terms of a complete set of eigenstates of $\hat{H}_0$ inserted between each term. With the redefinition $\epsilon\hbar\equiv\varepsilon$, one arrives at the time-independent power series expansion of the S-matrix

$$\begin{aligned}\text{Lim}_{\varepsilon\to 0}\,\langle\psi_f|\hat{S}_\varepsilon|\psi_i\rangle=\langle\psi_f|\psi_i\rangle-\text{Lim}_{\varepsilon\to 0}\,2\pi i\delta(E_f-E_0)\times\\ \langle\psi_f|\hat{H}_1\sum_{n=0}^{\infty}\left(\frac{1}{E_0-\hat{H}_0+i\varepsilon}\hat{H}_1\right)^n|\psi_i\rangle\end{aligned}\tag{4.53}$$

Several comments:

- The $n=0$ term is exactly Fermi's Golden Rule (see Vol. I);
- The $+i\varepsilon$ in the denominator, with the sign coming from the correct convergence factor in the integrals, just determines the correct *boundary conditions* to put in the Green's function (see later);
- We have proceeded to take the $\varepsilon\to 0$ limit in the final factor

$$\text{Lim}_{\,\epsilon\to 0}\int_{-\infty}^{\infty}dx_1\,e^{\{\frac{i}{\hbar}(E_f-E_0)x_1-\epsilon|x_1|\}}=2\pi\hbar\,\delta(E_f-E_0)\tag{4.54}$$

- The T-matrix can now be identified from Eqs. (4.41) and (4.53)

$$\begin{aligned}\tilde{T}_{fi}&\equiv\langle\psi_f|\hat{T}|\psi_i\rangle\\ \langle\psi_f|\hat{T}|\psi_i\rangle&=\langle\psi_f|\hat{H}_1\sum_{n=0}^{\infty}\left(\frac{1}{E_0-\hat{H}_0+i\varepsilon}\hat{H}_1\right)^n|\psi_i\rangle\quad;\ \text{T-matrix}\end{aligned}\tag{4.55}$$

- This last relation can be rewritten as

$$\langle\psi_f|\hat{T}|\psi_i\rangle = \langle\psi_f|\hat{H}_1|\psi_i^{(+)}\rangle$$
$$|\psi_i^{(+)}\rangle \equiv \sum_{n=0}^{\infty}\left(\frac{1}{E_0-\hat{H}_0+i\varepsilon}\hat{H}_1\right)^n|\psi_i\rangle \qquad (4.56)$$

We show below that this is indeed identical to the state $|\psi_i^{(+)}\rangle$ previously introduced in Eq. (4.33). If the first term is separated out in Eq. (4.56), and the series for $|\psi_i^{(+)}\rangle$ again identified in the second, this relation can be rewritten as

$$|\psi_i^{(+)}\rangle = |\psi_i\rangle + \frac{1}{E_0-\hat{H}_0+i\varepsilon}\hat{H}_1|\psi_i^{(+)}\rangle \quad ; \text{ Lippmann-Schwinger} \quad (4.57)$$

In this form, when projected into the coordinate representation, one has an *integral equation* for $|\psi_i^{(+)}\rangle$. This is the *Lippmann-Schwinger equation* [Lippmann and Schwinger (1950)], which has a meaning that extends beyond the power series expansion though which it has been derived. Note that from Eq. (4.57), one observes

$$(E_0-\hat{H}_0)|\psi_i^{(+)}\rangle = \hat{H}_1|\psi_i^{(+)}\rangle$$
$$\text{or} \qquad (E_0-\hat{H})|\psi_i^{(+)}\rangle = 0 \qquad ; \Omega\to\infty,\ \varepsilon\to 0 \qquad (4.58)$$

Thus the state $|\psi_i^{(+)}\rangle$, in the limits as the quantization volume $\Omega\to\infty$, and as the adiabatic damping factor $\varepsilon\to 0$, is a scattering state that is an *eigenstate of the full $\hat{H}$ with eigenvalue E_0*.[11] This is the same energy we started with at $t\to-\infty$ in the interaction picture.

- One therefore does not generate all of the eigenstates of $\hat{H}$ in this manner, if there are bound states, but only the continuum scattering states.[12]
- The terms with $n\geq 1$ in Eq. (4.56) give the *higher Born approximations* for the scattering amplitude. This is just "old-fashioned" perturbation theory, except that with the $+i\varepsilon$ in them, *we now know what to do when the denominators vanish.*
- People tried to do QED with this perturbation scheme; however, by singling out the time integration, the scattering amplitude is no longer

[11] Although the dependence on Ω is not explicit, we know, for example, that with a potential $V(r)$ in a big box with rigid walls there will be a finite shift in the energy levels as the interaction is turned on; this energy shift only vanishes in the limit $\Omega\to\infty$.

[12] The completeness relation is now $\sum_i|\psi_i^{(+)}\rangle\langle\psi_i^{(+)}| + \sum_{\text{bnd states}}|\psi_b\rangle\langle\psi_b| = \hat{1}$.

explicitly covariant. Infinities arise from various sources, which are not interpretable in a non-covariant approach. We will find that by leaving the time integrations in, and starting from Eq. (4.17), we are able to maintain a covariant, gauge-invariant S-matrix, which proves essential to developing a consistent renormalization scheme.[13]

4.7 Scattering State

The *Heisenberg picture* for the state vector is defined as follows

$$|\Psi_{\rm H}\rangle \equiv e^{\frac{i}{\hbar}\hat{H}t}\,|\Psi(t)\rangle \qquad ;\ \text{Heisenberg picture} \tag{4.59}$$

Correspondingly, an operator in the Heisenberg picture is defined by

$$\hat{O}_{\rm H} \equiv e^{\frac{i}{\hbar}\hat{H}t}\,\hat{O}\,e^{-\frac{i}{\hbar}\hat{H}t} \qquad ;\ \text{Heisenberg picture} \tag{4.60}$$

It follows from Eq. (4.32) that the Heisenberg state vector is independent of time[14]

$$i\hbar\frac{\partial}{\partial t}|\Psi_{\rm H}\rangle = 0 \tag{4.61}$$

The interaction-picture state vector is defined in Eq. (4.2). The state vectors in all the different pictures *coincide* at $t = 0$

$$|\Psi_{\rm H}\rangle = |\Psi(0)\rangle = |\Psi_{\rm I}(0)\rangle \tag{4.62}$$

This provides further motivation for looking at the scattering state $|\psi_i^{(+)}\rangle$ defined in Eq. (4.33) by

$$|\psi_i^{(+)}\rangle \equiv \hat{U}_\epsilon(0,-\infty)|\psi_i\rangle \tag{4.63}$$

The nth order contribution to $\hat{U}_\varepsilon(0,-\infty)$ explicitly contains n powers of $\hat{H}_1$

$$\hat{U}_\epsilon^{(n)}(0,-\infty)|\psi_i\rangle = \left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{0} e^{\epsilon t_1}\,dt_1 \int_{-\infty}^{t_1} e^{\epsilon t_2}\,dt_2 \cdots \int_{-\infty}^{t_{n-1}} e^{\epsilon t_n}\,dt_n \times$$
$$e^{\frac{i}{\hbar}\hat{H}_0 t_1}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0(t_1-t_2)}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0(t_2-t_3)}\cdots e^{-\frac{i}{\hbar}\hat{H}_0(t_{n-1}-t_n)}\hat{H}_1 e^{-\frac{i}{\hbar}\hat{H}_0 t_n}|\psi_i\rangle \tag{4.64}$$

[13] See the discussion in Vol. I.

[14] We remind the reader of the assumption, at this point, that $\hat{H}$ has no explicit time dependence.

In comparing with our starting point in Eq. (4.47) from which we proceeded to explicitly carrying out the time integrations, we note two differences:

- All the times satisfy $t \leq 0$, hence the adiabatic damping factors in all cases become $e^{-\epsilon|t|} = e^{\epsilon t}$;
- There is no eigenstate $|\psi_f\rangle$ on the left, and hence the operator $\hat{H}_0$ on the left can no longer be replaced by its eigenvalue E_f.

We may proceed to change variables as in Eqs. (4.48)–(4.50). This time, instead of $e^{-\epsilon|x_1+x_2+\cdots+x_n|}$, for example, we have $e^{\epsilon(x_1+x_2+\cdots+x_n)}$ so that all the adiabatic damping factors can simply be moved to their appropriate position in the multiple integral. Thus we arrive at

$$\hat{U}_\epsilon^{(n)}(0,-\infty)|\psi_i\rangle = \left(-\frac{i}{\hbar}\right)^n \int_{-\infty}^{0} dx_1\, e^{n\epsilon x_1} e^{\frac{i}{\hbar}(\hat{H}_0-E_0)x_1}\, \hat{H}_1 \times$$
$$\int_{-\infty}^{0} dx_2\, e^{(n-1)\epsilon x_2} e^{\frac{i}{\hbar}(\hat{H}_0-E_0)x_2}\, \hat{H}_1 \int_{-\infty}^{0} dx_3\, e^{(n-2)\epsilon x_3} e^{\frac{i}{\hbar}(\hat{H}_0-E_0)x_3}\, \hat{H}_1 \times \cdots$$
$$\cdots \hat{H}_1 \int_{-\infty}^{0} dx_n\, e^{\epsilon x_n} e^{\frac{i}{\hbar}(\hat{H}_0-E_0)x_n}\, \hat{H}_1 |\psi_i\rangle \tag{4.65}$$

All the integrals now *explicitly factor*, and they can immediately be done just as before with the result

$$\hat{U}_\varepsilon^{(n)}(0,-\infty)|\psi_i\rangle = \frac{1}{E_0-\hat{H}_0+in\varepsilon}\hat{H}_1 \frac{1}{E_0-\hat{H}_0+i(n-1)\varepsilon}\hat{H}_1 \cdots$$
$$\cdots \frac{1}{E_0-\hat{H}_0+i\varepsilon}\hat{H}_1|\psi_i\rangle \tag{4.66}$$

Again, we are interested in the limit as $\varepsilon \to 0$. Each of the $i\bar{n}\varepsilon$ in the denominators, where $\bar{n} = (1, 2, \cdots, n)$, simply serves to define how one treats the singularity in the individual Green's functions.[15] Hence, we can simply *replace them all by $i\varepsilon$ in the limit.* Thus we indeed reproduce the previously employed expression in Eq. (4.56)

$$|\psi_i^{(+)}\rangle = \hat{U}_\varepsilon(0,-\infty)|\psi_i\rangle$$
$$= \sum_{n=0}^{\infty} \left(\frac{1}{E_0-\hat{H}_0+i\varepsilon}\hat{H}_1\right)^n |\psi_i\rangle \qquad ;\ \text{scattering state} \tag{4.67}$$

Again, by separating out the first term in the second line, and then re-

[15] They serve to define a contour in the evaluation of the Green's functions (see later).

identifying the series for $|\psi_i^{(+)}\rangle$, this can be rewritten as an integral equation

$$|\psi_i^{(+)}\rangle = |\psi_i\rangle + \frac{1}{E_0 - \hat{H}_0 + i\varepsilon}\hat{H}_1|\psi_i^{(+)}\rangle \tag{4.68}$$

and the integral equation has a meaning, even when the power series solution to it does not.

Let us also consider the fully interacting state $|\psi_f^{(-)}\rangle \equiv |\Psi_{\rm I}^f(0)\rangle$ that as $t \to +\infty$ reduces to the state $|\psi_f\rangle$, so that $|\psi_f^{(-)}\rangle = \hat{U}_\epsilon(0, +\infty)|\psi_f\rangle$. If we go back to Eq. (4.19), and go through the arguments leading from Eq. (4.64) to (4.67), we see that the only changes are the replacements $E_0 \to E_f$ and $\varepsilon \to -\varepsilon$ (see Prob. 4.3). Thus

$$\begin{aligned} |\psi_f^{(-)}\rangle &\equiv \hat{U}_\varepsilon(0, +\infty)|\psi_f\rangle \\ &= \sum_{n=0}^{\infty}\left(\frac{1}{E_f - \hat{H}_0 - i\varepsilon}\hat{H}_1\right)^n |\psi_f\rangle \quad ; \text{ scattering state} \end{aligned} \tag{4.69}$$

This can again be written as an integral equation, which has meaning even when the power series solution for it does not

$$|\psi_f^{(-)}\rangle = |\psi_f\rangle + \frac{1}{E_f - \hat{H}_0 - i\varepsilon}\hat{H}_1|\psi_f^{(-)}\rangle \tag{4.70}$$

The state $|\psi^{(+)}\rangle$ is known as the *outgoing* scattering state, and $|\psi^{(-)}\rangle$ as the *incoming* scattering state.[16]

There are some important properties of these scattering states that follow immediately:

(1) The unitarity of the $\hat{U}_\varepsilon$ operator implies that

$$\langle\psi_{i'}^{(+)}|\psi_i^{(+)}\rangle = \langle\psi_{i'}|\hat{U}_\varepsilon(0, -\infty)^\dagger\hat{U}_\varepsilon(0, -\infty)|\psi_i\rangle = \langle\psi_{i'}|\psi_i\rangle = \delta_{i'i} \tag{4.71}$$

Similarly[17]

$$\langle\psi_{f'}^{(-)}|\psi_f^{(-)}\rangle = \delta_{f'f} \tag{4.72}$$

[16]The Green's function in the former case has outgoing scattered waves, while in the latter case they are incoming [compare Eq. (4.107) and Prob. 4.9].

[17]The completeness relation can also be written $\sum_f |\psi_f^{(-)}\rangle\langle\psi_f^{(-)}| + \sum_{\text{bnd states}} |\psi_b\rangle\langle\psi_b| = \hat{1}$.

(2) Furthermore, from Eq. (4.21) and the group property of $\hat{U}_\varepsilon$, it follows that

$$\begin{aligned}\langle\psi_f^{(-)}|\psi_i^{(+)}\rangle &= \langle\psi_f|\hat{U}_\varepsilon(0,+\infty)^\dagger\hat{U}_\varepsilon(0,-\infty)|\psi_i\rangle \\ &= \langle\psi_f|\hat{U}_\varepsilon(+\infty,0)\hat{U}_\varepsilon(0,-\infty)|\psi_i\rangle \\ &= \langle\psi_f|\hat{U}_\varepsilon(+\infty,-\infty)|\psi_i\rangle \end{aligned} \tag{4.73}$$

Thus the inner product of $|\psi_f^{(-)}\rangle$ and $|\psi_i^{(+)}\rangle$ is just the S-matrix!

$$\langle\psi_f^{(-)}|\psi_i^{(+)}\rangle = \langle\psi_f|\hat{S}|\psi_i\rangle \qquad ;\ S\text{-matrix} \tag{4.74}$$

(3) Since taking the adjoint merely reverses the order of the operators and changes the sign of the $i\varepsilon$, the T-matrix in Eq. (4.55) can also be written in the case $E_f = E_0$ as

$$\begin{aligned}\langle\psi_f|\hat{T}|\psi_i\rangle &= \langle\psi_f|\hat{H}_1\sum_{n=0}^{\infty}\left(\frac{1}{E_0-\hat{H}_0+i\varepsilon}\hat{H}_1\right)^n|\psi_i\rangle \\ &= \langle\psi_f|\left[\sum_{n=0}^{\infty}\left(\frac{1}{E_0-\hat{H}_0-i\varepsilon}\hat{H}_1\right)^n\right]^\dagger\hat{H}_1|\psi_i\rangle \\ &= \langle\psi_f^{(-)}|\hat{H}_1|\psi_i\rangle \qquad ;\ E_f = E_0 \end{aligned} \tag{4.75}$$

(4) Thus, in *summary*, in addition to the explicit power-series expansions in Eqs. (4.53) and (4.55), we have expressions for the S-matrix and T-matrix in terms of the incoming and outgoing scattering states that are more general than the power-series solutions through which they were derived

$$\begin{aligned}\langle\psi_f|\hat{S}|\psi_i\rangle &= \langle\psi_f^{(-)}|\psi_i^{(+)}\rangle \qquad ;\ S\text{-matrix} \\ &= \langle\psi_f|\psi_i\rangle - 2\pi i\delta(E_f-E_0)\langle\psi_f|\hat{T}|\psi_i\rangle \\ \langle\psi_f|\hat{T}|\psi_i\rangle &= \langle\psi_f|\hat{H}_1|\psi_i^{(+)}\rangle = \langle\psi_f^{(-)}|\hat{H}_1|\psi_i\rangle \qquad ;\ T\text{-matrix} \end{aligned} \tag{4.76}$$

4.8 Transition Rate

We now calculate the transition rate directly, in the presence of the adiabatic switching. The derivation is from [Gell-Mann and Goldberger (1953)], in their classic paper on scattering theory. The only subtlety in the calculation is identifying those expressions that are well-defined in the limit $\varepsilon \to 0$, and knowing when to take that limit. This takes a little experience.

The Schrödinger state vector at the finite time t for a system that started as $|\psi_i\rangle$ at $t \to -\infty$ is

$$|\Psi_i(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\Psi_i(0)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}\hat{U}_\varepsilon(0,-\infty)|\psi_i\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi_i^{(+)}\rangle \quad (4.77)$$

The states that one *observes experimentally* in scattering, decays, *etc.* are the free-particle states

$$|\Phi_f(t)\rangle = e^{-\frac{i}{\hbar}E_f t}|\psi_f\rangle \quad (4.78)$$

From the general principles of quantum mechanics, the probability of finding the system in the state $|\Phi_f(t)\rangle$ at the time t, if it started in $|\psi_i\rangle$ at $t \to -\infty$, is then

$$P_{fi}(t) = |\langle\Phi_f(t)|\Psi_i(t)\rangle|^2 \equiv |M_{fi}(t)|^2 \quad (4.79)$$

This is the probability of having made a transition to the state $|\Phi_f(t)\rangle$ at the time t. The transition *rate* is the time derivative of this quantity

$$\omega_{fi} = \frac{d}{dt}P_{fi}(t) = M_{fi}^\star(t)\frac{d}{dt}M_{fi}(t) + \text{c.c.} \quad (4.80)$$

We will show that this transition rate is independent of time for times such that $|t| \ll 1/\varepsilon$. In the end, we will again let $\Omega \to \infty$, and $\varepsilon \to 0$, where Ω is the quantization volume. Let us proceed to calculate the transition rate.

From Eqs. (4.77)–(4.79) one has

$$\begin{aligned} M_{fi}(t) &= \langle\Phi_f(t)|\Psi_i(t)\rangle \\ &= \langle\psi_f|e^{\frac{i}{\hbar}E_f t}e^{-\frac{i}{\hbar}\hat{H}t}|\psi_i^{(+)}\rangle \end{aligned} \quad (4.81)$$

This relation may be differentiated with respect to time to give

$$\frac{d}{dt}M_{fi}(t) = -\frac{i}{\hbar}\langle\psi_f|(\hat{H}-E_f)e^{\frac{i}{\hbar}E_f t}e^{-\frac{i}{\hbar}\hat{H}t}|\psi_i^{(+)}\rangle \quad (4.82)$$

The observation that $(\hat{H}-E_f)|\psi_f\rangle = (\hat{H}_0+\hat{H}_1-E_f)|\psi_f\rangle = \hat{H}_1|\psi_f\rangle$ gives

$$\frac{d}{dt}M_{fi}(t) = -\frac{i}{\hbar}e^{\frac{i}{\hbar}E_f t}\langle\psi_f|\hat{H}_1\, e^{-\frac{i}{\hbar}\hat{H}t}|\psi_i^{(+)}\rangle \quad (4.83)$$

Now Eq. (4.58) states that in the above limit

$$(E_0-\hat{H})|\psi_i^{(+)}\rangle = 0 \qquad ;\ \begin{matrix}\Omega \to \infty \\ \varepsilon \to 0\end{matrix} \quad (4.84)$$

Use of this relation in Eqs. (4.83) and (4.81) then gives

$$\frac{d}{dt}M_{fi}(t) = -\frac{i}{\hbar}e^{\frac{i}{\hbar}(E_f-E_0)t}\langle\psi_f|\hat{H}_1|\psi_i^{(+)}\rangle$$
$$M_{fi}(t) = e^{\frac{i}{\hbar}(E_f-E_0)t}\langle\psi_f|\psi_i^{(+)}\rangle \tag{4.85}$$

Substitution of these relations into Eq. (4.80) then expresses the transition rate as

$$\omega_{fi} = \frac{2}{\hbar}\mathrm{Im}\,\langle\psi_f|\hat{H}_1|\psi_i^{(+)}\rangle\langle\psi_f|\psi_i^{(+)}\rangle^\star \tag{4.86}$$

This expression now has the following properties:

- It is independent of time;
- It is *well-defined in the limit* $\Omega \to \infty$, $\varepsilon \to 0$.[18]

From our previous analysis in Eqs. (4.76) and (4.68), we have

$$\langle\psi_f|\hat{H}_1|\psi_i^{(+)}\rangle = \langle\psi_f|\hat{T}|\psi_i\rangle = \tilde{T}_{fi}$$
$$|\psi_i^{(+)}\rangle = |\psi_i\rangle + \frac{1}{E_0 - \hat{H}_0 + i\varepsilon}\hat{H}_1|\psi_i^{(+)}\rangle \tag{4.87}$$

The inner product of the second relation with $|\psi_f\rangle$ gives

$$\langle\psi_f|\psi_i^{(+)}\rangle = \langle\psi_f|\psi_i\rangle + \frac{1}{E_0 - E_f + i\varepsilon}\tilde{T}_{fi} \tag{4.88}$$

Substitution of this relation and the first of Eqs. (4.87) into Eq. (4.86) then gives

$$\omega_{fi} = \frac{2}{\hbar}\delta_{fi}\,\mathrm{Im}\,\tilde{T}_{ii} + \frac{2}{\hbar}\mathrm{Im}\,\frac{1}{E_0 - E_f - i\varepsilon}|\tilde{T}_{fi}|^2 \tag{4.89}$$

Finally, we make use of the relation

$$\frac{1}{E_0 - E_f - i\varepsilon} = \mathcal{P}\frac{1}{E_0 - E_f} + i\pi\delta(E_0 - E_f) \tag{4.90}$$

Here $\mathcal{P}$ denotes the Cauchy principal value, defined by deleting an infinitesimal symmetric region of integration through the singularity, and then letting the size of that region go to zero. Equation (4.90) is a statement on

[18] Here we will simply justify this observation *a posteriori*, through the many applications of the final expression. Note that by taking this limit too early in the derivation, one can arrive at spurious results [for example, try substituting the second of Eqs. (4.85) into Eq. (4.79)].

contour integration; it is derived in Prob. B.4. With the use of this relation, Eqs. (4.89) and (4.76) become

$$\begin{aligned} \omega_{fi} &= \frac{2}{\hbar}\delta_{fi}\,\mathrm{Im}\,\tilde{T}_{ii} + \frac{2\pi}{\hbar}\delta(E_0 - E_f)|\tilde{T}_{fi}|^2 \quad ;\ \text{transition rate} \\ S_{fi} &= \delta_{fi} - 2\pi i\delta(E_0 - E_f)\tilde{T}_{fi} \qquad\qquad ;\ S\text{-matrix} \end{aligned} \tag{4.91}$$

These expressions are exact. They are the results quoted in Eqs. (4.46) and used extensively in Vol. I.

4.9 Unitarity

The first term on the r.h.s. of ω_{fi} in Eq. (4.91) only contributes if $f = i$; it is there to take into account the depletion of the initial state. Return to Eq. (4.79). With the completeness of the states $|\Phi_f(t)\rangle$, and the normalization of the state $|\Psi_i(t)\rangle$, a sum over all final states gives[19]

$$\begin{aligned} \sum_f P_{fi}(t) &= \sum_f \langle\Psi_i(t)|\Phi_f(t)\rangle\langle\Phi_f(t)|\Psi_i(t)\rangle \\ &= \langle\Psi_i(t)|\Psi_i(t)\rangle = 1 \end{aligned} \tag{4.92}$$

This is the statement of conservation of probability—the initial state must end up *somewhere*. The time derivative of this sum then vanishes

$$\frac{d}{dt}\sum_f P_{fi}(t) = \sum_f \frac{d}{dt}P_{fi}(t) = \sum_f \omega_{fi} = 0 \tag{4.93}$$

Here the transition rate has been identified from Eq. (4.80). A substitution of the expression for the transition rate in Eq. (4.91) into this relation then gives

$$-\frac{2}{\hbar}\mathrm{Im}\,\tilde{T}_{ii} = \sum_f \frac{2\pi}{\hbar}\delta(E_f - E_0)|\tilde{T}_{fi}|^2 \qquad ;\ \text{unitarity} \tag{4.94}$$

This relation for the imaginary part of the elastic T-matrix, reflecting conservation of probability and depletion of the initial state, is known as *unitarity*.

[19] This sum now *includes* the state $f = i$; the reader should note that there is no sum over the repeated index i implied in Eqs. (4.91) and (4.94).

4.10 Example: Potential Scattering

To see one practical application of the preceding scattering theory, consider the elastic scattering of a non-relativistic particle of mass m from a spherically symmetric potential $\hat{H}_1 = V(|\hat{\mathbf{x}}|)$ in three dimensions. First we calculate the Green's function, or propagator.

4.10.1 *Green's Function (Propagator)*

The Green's function in this case is defined by the following matrix element taken between eigenstates of position

$$G_0(\mathbf{x}-\mathbf{y}) = \langle \mathbf{x}| \frac{1}{\hat{H}_0 - E_0 - i\varepsilon} |\mathbf{y}\rangle \qquad ;\ \text{Green}'\text{s function} \tag{4.95}$$

Here

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} \qquad ;\ E_0 \equiv \frac{\hbar^2 \mathbf{k}^2}{2m} \tag{4.96}$$

As usual, we start in a big cubical box of volume Ω where the eigenstates of momentum are plane waves satisfying periodic boundary conditions

$$\begin{aligned} \hat{\mathbf{p}}\,|\mathbf{t}\rangle &= \hbar \mathbf{t}\,|\mathbf{t}\rangle \\ \langle \mathbf{x}|\mathbf{t}\rangle &= \phi_{\mathbf{t}}(\mathbf{x}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{t}\cdot\mathbf{x}} \qquad ;\ \text{p.b.c.} \end{aligned} \tag{4.97}$$

The eigenstates of momentum satisfy the completeness relation

$$\sum_{\mathbf{t}} |\mathbf{t}\rangle\langle\mathbf{t}| = \hat{1} \tag{4.98}$$

Insert this expression in Eq. (4.95), and use Eqs. (4.96) and (4.97)

$$\begin{aligned} G_0(\mathbf{x}-\mathbf{y}) &= \frac{2m}{\hbar^2} \sum_{\mathbf{t}} \langle \mathbf{x}|\mathbf{t}\rangle \frac{1}{t^2 - k^2 - i\varepsilon} \langle \mathbf{t}|\mathbf{y}\rangle \\ &= \frac{2m}{\hbar^2} \frac{1}{\Omega} \sum_{\mathbf{t}} e^{i\mathbf{t}\cdot(\mathbf{x}-\mathbf{y})} \frac{1}{t^2 - k^2 - i\varepsilon} \end{aligned} \tag{4.99}$$

We have redefined $(2m/\hbar^2)\varepsilon \to \varepsilon$ in this expression.

Now take the limit as the volume $\Omega \to \infty$, in which case the sum over states becomes an integral, in the familiar fashion, $\sum_{\mathbf{t}} \to \Omega(2\pi)^{-3} \int d^3t$. In this limit

$$G_0(\mathbf{x}-\mathbf{y}) = \frac{2m}{\hbar^2} \frac{1}{(2\pi)^3} \int d^3t\ e^{i\mathbf{t}\cdot(\mathbf{x}-\mathbf{y})} \frac{1}{t^2 - k^2 - i\varepsilon} \tag{4.100}$$

It remains to do this integral. Take $\mathbf{r} \equiv \mathbf{x} - \mathbf{y}$ to define the z-axis. Then $\mathbf{t} \cdot (\mathbf{x} - \mathbf{y}) = tr\cos\theta$ and $d^3t = t^2 dt\, d\phi \sin\theta\, d\theta$. The angular integrations are then immediately performed

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, e^{itr\cos\theta} = 2\pi \int_{-1}^{1} dx\, e^{itrx} = 4\pi \frac{\sin tr}{tr} \tag{4.101}$$

We are left with

$$G_0(\mathbf{x} - \mathbf{y}) = \frac{2m}{\hbar^2} \frac{4\pi}{(2\pi)^3} \frac{1}{r} \int_0^{\infty} tdt\, \sin tr \frac{1}{t^2 - k^2 - i\varepsilon} \tag{4.102}$$

Now write the integral as

$$\begin{aligned} \int_0^{\infty} tdt\, \sin tr \cdots &= \int_0^{\infty} tdt\, \frac{1}{2i}(e^{itr} - e^{-itr}) \cdots \\ &= \frac{1}{2i} \int_{-\infty}^{\infty} tdt\, e^{itr} \cdots \end{aligned} \tag{4.103}$$

Here we have simple changed variables $t \to -t$ in the second term, and combined it with the first (the rest of the integrand is a function of t^2). The required integral is then reduced to

$$G_0(\mathbf{x} - \mathbf{y}) = \frac{2m}{\hbar^2} \frac{4\pi}{(2\pi)^3} \frac{1}{2ir} \int_{-\infty}^{\infty} tdt\, e^{itr} \frac{1}{t^2 - k^2 - i\varepsilon} \quad ;\ \mathbf{r} \equiv \mathbf{x} - \mathbf{y} \tag{4.104}$$

where the integral now runs along the entire real t-axis. There is sufficient convergence in the integrand that closing the contour with a semi-circle in the upper-1/2 t-plane makes a vanishing contribution to the integral in the limit as the radius R of that semi-circle becomes infinite.[20] Thus the free Green's function has been reduced to a *contour integral* where the contour C is that illustrated in Fig. 4.1.

The integral is then evaluated using the complex-variable techniques summarized in appendix B. The integrand is an analytic function of t except at the poles where the denominator vanishes. That denominator can be rewritten as

$$\frac{1}{t^2 - k^2 - i\varepsilon} = \frac{1}{(t - k - i\varepsilon)(t + k + i\varepsilon)} \tag{4.105}$$

where we have again redefined $\varepsilon \to 2k\varepsilon$ (here $k > 0$), and neglected $O(\varepsilon^2)$. The integrand thus has simple poles at $t = k + i\varepsilon$ and $t = -k - i\varepsilon$, only the first of which lies inside C.

[20] See Prob. 4.4.

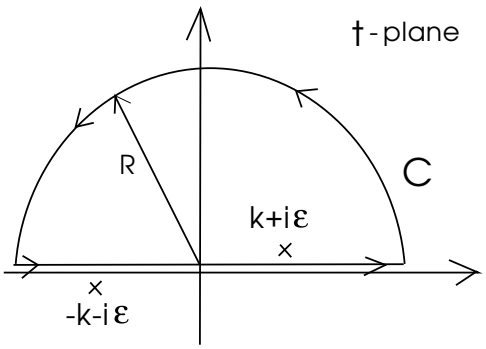

Fig. 4.1 Contour for the evaluation of the Green's function $G_0(\mathbf{x}-\mathbf{y})$ in the complex t-plane, together with the singularity structure arrived at with adiabatic damping. Here $R \to \infty$.

The integral is then given by $2\pi i \times$ (residue at k). Thus

$$G_0(\mathbf{x}-\mathbf{y}) = \frac{2m}{\hbar^2}\frac{4\pi}{(2\pi)^3}\frac{1}{2ir}2\pi i\left(\frac{e^{ikr}}{2}\right) \tag{4.106}$$

Hence we arrive at our final result for the free Green's function in potential scattering

$$G_0(\mathbf{x}-\mathbf{y}) = \frac{2m}{\hbar^2}\frac{e^{ikr}}{4\pi r} \qquad ;\ \mathbf{r} \equiv \mathbf{x}-\mathbf{y} \tag{4.107}$$

This is recognized as the familiar Green's function for the scalar Helmholtz equation (see [Fetter and Walecka (2003)]).

4.10.2 *Scattering Wave Function*

The scattering state $|\psi_i^{(+)}\rangle$ can be similarly projected onto eigenstates of position. With the use of the completeness relation for these eigenstates, and the definition of the Green's function in Eq. (4.95), one has[21]

$$\langle \mathbf{x}|\psi_i^{(+)}\rangle = \langle \mathbf{x}|\psi_i\rangle - \int d^3y\, \langle \mathbf{x}|\frac{1}{\hat{H}_0 - E_0 - i\varepsilon}|\mathbf{y}\rangle\, V(y)\, \langle \mathbf{y}|\psi_i^{(+)}\rangle \tag{4.108}$$

With the definition $\langle \mathbf{x}|\psi_i^{(+)}\rangle \equiv \psi_i^{(+)}(\mathbf{x})/\sqrt{\Omega}$, this becomes an integral equation for the scattering wave function

$$\begin{aligned} \langle \mathbf{x}|\psi_i^{(+)}\rangle &\equiv \frac{1}{\sqrt{\Omega}}\psi_i^{(+)}(\mathbf{x}) \\ \psi_i^{(+)}(\mathbf{x}) &= e^{i\mathbf{k}\cdot\mathbf{x}} - \int d^3y\, G_0(\mathbf{x}-\mathbf{y})\, V(y)\, \psi_i^{(+)}(\mathbf{y}) \end{aligned} \tag{4.109}$$

[21] We have used $V(|\hat{\mathbf{x}}|)\,|\mathbf{y}\rangle = V(y)\,|\mathbf{y}\rangle$ where $y \equiv |\mathbf{y}|$; note the sign of the second term.

4.10.3 *T-matrix*

The T-matrix can also be expressed in the coordinate representation as

$$\tilde{T}_{fi} = \int d^3y \, \langle \mathbf{k}_f | \mathbf{y} \rangle \, V(y) \, \langle \mathbf{y} | \psi_i^{(+)} \rangle \tag{4.110}$$

where the final state is now written explicitly as an eigenstate of momentum $|\psi_f\rangle \equiv |\mathbf{k}_f\rangle$. With the introduction of the corresponding wave functions, one has

$$\tilde{T}_{fi} = \frac{1}{\Omega} \int d^3y \, e^{-i\mathbf{k}_f \cdot \mathbf{y}} \, V(y) \, \psi_i^{(+)}(\mathbf{y}) \tag{4.111}$$

4.10.4 *Cross Section*

The differential cross section follows from the transition rate according to Eq. (4.45)

$$d\sigma = \frac{2\pi}{\hbar} \delta(E_f - E_0) |\tilde{T}_{fi}|^2 \frac{dn_f}{I_{\text{inc}}} \tag{4.112}$$

In this expression:

(1) The incident wave function is $\psi_i(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}/\sqrt{\Omega}$. This yields an incident probability flux of

$$I_{\text{inc}} = \frac{1}{\Omega} \frac{\hbar k}{m} \tag{4.113}$$

(2) The number of final states in a big box with periodic boundary conditions is

$$dn_f = \frac{\Omega}{(2\pi)^3} d^3k_f = \frac{\Omega}{(2\pi)^3} k_f^2 dk_f \, d\Omega_f \tag{4.114}$$

(3) The integral over the energy-conserving delta function gives

$$\int \delta(E_f - E_0) k_f^2 dk_f = \frac{2m}{\hbar^2} \frac{k_f}{2} \qquad ; \; |\mathbf{k}_f| = |\mathbf{k}| \tag{4.115}$$

(4) A combination of the results in Eqs. (4.112)–(4.115) gives

$$\frac{d\sigma}{d\Omega_f} = \frac{2\pi}{\hbar} \left[\frac{\Omega}{(2\pi)^3} \frac{mk}{\hbar^2} \right] \left[\frac{\Omega m}{\hbar k} \right] |\tilde{T}_{fi}|^2 \tag{4.116}$$

The factors of Ω cancel, as they must, and the final result for the differential cross section for elastic scattering of a particle of energy

$E_0 = \hbar^2 k^2/2m$ from the potential $V(|\mathbf{x}|)$ takes the form

$$\frac{d\sigma}{d\Omega_f} = |f(k,\theta)|^2$$

$$f(k,\theta) \equiv -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3y\, e^{-i\mathbf{k}_f\cdot\mathbf{y}}\, V(y)\, \psi_i^{(+)}(\mathbf{y}) \qquad (4.117)$$

The minus sign is conventional.

(5) The scattering wave function $\psi_i^{(+)}(\mathbf{x})$ in this expression is the solution to the integral equation

$$\psi_i^{(+)}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{2m}{\hbar^2}\int d^3y\, \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}\, V(y)\, \psi_i^{(+)}(\mathbf{y}) \qquad (4.118)$$

4.10.5 *Unitarity*

The scattering amplitude $f(k,\theta)$ and the T-matrix are related through Eqs. (4.117) and (4.111), and thus

$$-\frac{2}{\hbar}\text{Im}\,\tilde{T}_{ii} = \frac{4\pi}{\Omega}\frac{\hbar}{m}\text{Im}\, f(k,0) \qquad (4.119)$$

The unitarity relation in Eq. (4.94) states that

$$-\frac{2}{\hbar}\text{Im}\,\tilde{T}_{ii} = \sum_f \frac{2\pi}{\hbar}\delta(E_f - E_0)|\tilde{T}_{fi}|^2 \qquad (4.120)$$

Within a factor of the incident flux, the r.h.s. of this relation is just the total cross section σ_{tot}. Thus Eq. (4.120) can be rewritten as

$$-\frac{2}{\hbar}\text{Im}\,\tilde{T}_{ii} = I_{\text{inc}}\,\sigma_{\text{tot}} = \frac{1}{\Omega}\frac{\hbar k}{m}\sigma_{\text{tot}} \qquad (4.121)$$

A comparison of Eqs. (4.119) and (4.121) then leads to the *optical theorem* relating the imaginary part of the forward elastic scattering amplitude and the total cross section[22]

$$\text{Im}\, f(k,0) = \frac{k}{4\pi}\sigma_{\text{tot}} \qquad ;\ \text{optical theorem} \qquad (4.122)$$

The analysis of potential scattering in this section provides the underlying basis for the study of scattering in quantum mechanics, as presented, for example, in [Schiff (1968)].[23]

[22] So far, there is only elastic scattering in this potential model, but the optical theorem is more general and holds in the presence of additional inelastic processes.

[23] Problems 1.1–1.5 in [Walecka (2004)] take the reader through the essentials of the partial-wave analysis of the scattering problem.