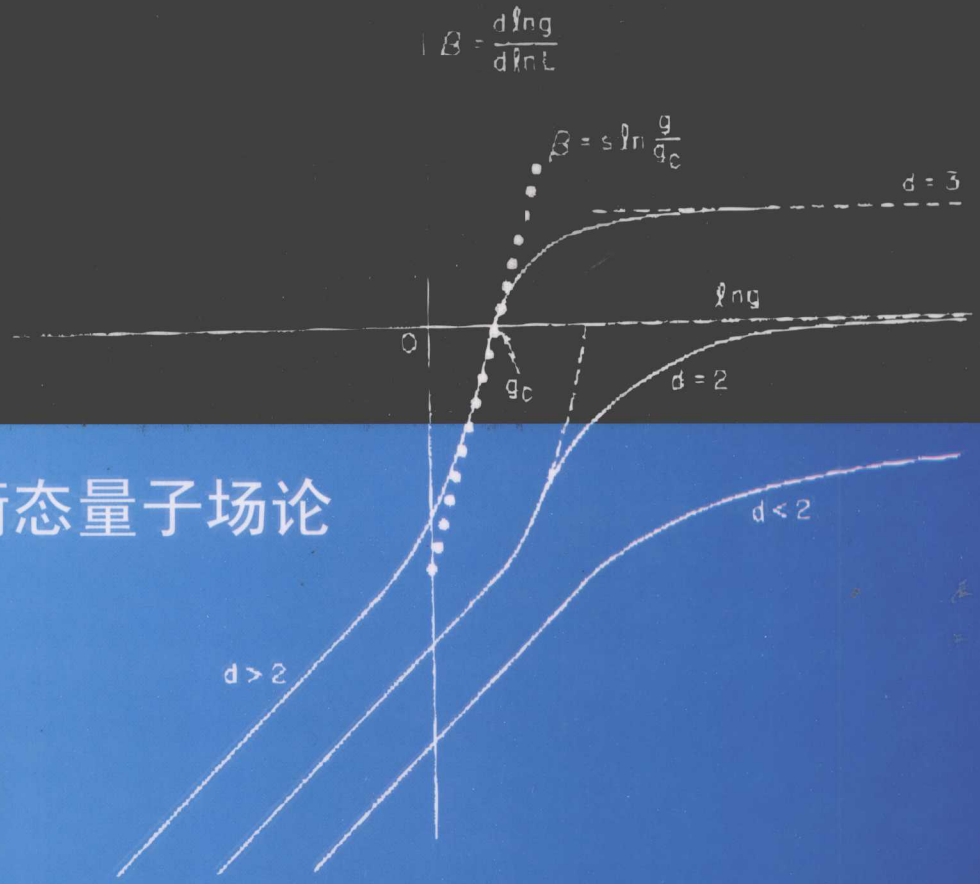
Jørgen Rammer

Quantum Field Theory of Non-equilibrium



非平衡态量子场论

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QUANTUM FIELD THEORY OF NON-EQUILIBRIUM STATES

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Preface

The purpose of this book is to provide an introduction to the applications of quantum field theoretic methods to systems out of equilibrium. The reason for adding a book on the subject of quantum field theory is two-fold: the presentation is, to my knowledge, the first to extensively present and apply to non-equilibrium phenomena the real-time approach originally developed by Schwinger, and subsequently applied by Keldysh and others to derive transport equations. Secondly, the aim is to show the universality of the method by applying it to a broad range of phenomena. The book should thus not just be of interest to condensed matter physicists, but to physicists in general as the method is of general interest with applications ranging the whole scale from high-energy to soft condensed matter physics. The universality of the method, as testified by the range of topics covered, reveals that the language of quantum fields is the universal description of fluctuations, be they of quantum nature, thermal or classical stochastic. The book is thus intended as a contribution to unifying the languages used in separate fields of physics, providing a universal tool for describing non-equilibrium states.

Chapter 1 introduces the basic notions of quantum field theory, the bose and fermi quantum fields operating on the multi-particle state spaces. In Chapter 2, operators on the multi-particle space representing physical quantities of a many-body system are constructed. The detailed exposition in these two chapters is intended to ensure the book is self-contained. In Chapter 3, the quantum dynamics of a many-body system is described in terms of its quantum fields and their correlation functions, the Green's functions. In Chapter 4, the key formal tool to describe non-equilibrium states is introduced: Schwinger's closed time path formulation of non-equilibrium quantum field theory, quantum statistical mechanics. Perturbation theory for non-equilibrium states is constructed starting from the canonical operator formalism presented in the previous chapters. In Chapter 5 we develop the real-time formalism necessary to deal with non-equilibrium states; first in terms of matrices and eventually in terms of two different types of Green's functions. The diagram representation of non-equilibrium perturbation theory is constructed in a way that the different aspects of spectral and quantum kinetic properties appear in a physically transparent and important fashion for non-equilibrium states. The equivalence of the real-time and imaginary-time formalisms are discussed in detail. In Chapter 6 we consider the coexistence regime between equilibrium and non-equilibrium states, the linear response regime. In Chapter 7 we develop and apply the quantum kinetic equation approach to the normal state, and in particular consider electrons

in metals and semiconductors. As applications we consider the Boltzmann limit, and then phenomena beyond the Boltzmann theory, such as renormalization of transport coefficients due to interactions. In Chapter 8 we consider non-equilibrium superconductivity. In particular we introduce the quasi-classical Green's function technique so efficient for the description of superfluids. We derive the quantum kinetic equation describing elastic and inelastic scattering in superconductors. The time-dependent Ginzburg–Landau equation is obtained for a dirty superconductor. As an application of the quasi-classical theory, we consider the phenomena of conversion of normal currents to supercurrents and the corresponding charge imbalance.

Unlike Schwinger, not stooping to the paganism of using diagrams, we shall, like the boys in the basement, take heavy advantage of using Feynman diagrams. By introducing Feynman diagrams, the most developed of our senses can become functional in the pursuit of understanding quantum dynamics, an addition that shall make its pursuit easier also for non-equilibrium situations. Though the picture of reality that the representation of perturbation theory in terms of Feynman diagrams inspires might be a figment of the imagination, its usefulness for developing physical intuition has amply proved its value, as witnessed first in elementary particle physics. We develop the diagrammatics for non-equilibrium states, and show that the additional rules for the universal vertex display the two important features of quantum statistics and spectral properties of the interacting particles in an explicit fashion. In Chapter 9 we shall take the stand of formulating the laws of physics in terms of propagators and vertices and their Feynman diagrams representing probability amplitudes as dictated by the superposition principle. In fact, we take the Shakespearian approach and construct quantum dynamics in terms of Feynman diagrams by invoking the only two options for a particle: *to act or not to interact.* From this diagrammatic starting point, and employing the intuitive appeal of diagrammatic arguments, we then construct the formalism of non-equilibrium quantum field theory in terms of the powerful functional methods; first in terms of the generating functional and functional differentiation technique. In Chapter 10 we then introduce the final tool in the functional arsenal: functional integration, and arrive at the effective action description of general non-equilibrium states. As an application of the effective action approach we consider the dilute Bose gas, and the case of a trapped Bose–Einstein condensate. In Chapter 11 we consider quantum transport properties of disordered conductors, weak localization and interaction effects. In particular we show how the quasi-classical Green's function technique used in describing non-equilibrium properties of a dirty superconductor can be utilized to describe the destruction of phase coherence in the normal state due to non-equilibrium effects and interactions. Finally, in Chapter 12, we consider the classical limit of the developed general non-equilibrium quantum field theory. We consider classical stochastic dynamics and show that field theoretic methods and diagrammatics are useful tools even in the classical context. As an example we consider the flux flow properties of the Abrikosov lattice in a type-II superconductor. We thus demonstrate the fact that quantum field theory, through its diagrammatics and functional formulations, is the universal language for describing fluctuations whatever their nature.

Readers' guide. Firstly, readers bothered by the old-fashioned habit of footnotes can simply skip them; they are either quick reminders or serve the purpose of pro-

viding a general perspective. The book can be read chronologically but, like any fox hole, it has two entrances. For the reader whose interest is the general structure of quantum field theories, the book offers the possibility to jump directly to Chapter 9 where a quantum field theory is defined in terms of its propagators and vertices and their resulting Feynman diagrams as dictated by the superposition principle. The powerful methods of generating functionals are then constructed from the diagrammatics. However, the reader acquainted with Chapter 4 will then have at hand the general quantum field theory applicable to non-equilibrium states.

The scope of the book is not so much to dwell on a detailed application of the non-equilibrium theory to a single topic, but rather to show the versatility and universality of the method by applying it to a broad range of core topics of physics. One purpose of the book is to demonstrate the utility of Feynman diagrams in non-equilibrium quantum statistical mechanics using an approach appealing to physical intuition. The real-time description of non-equilibrium quantum statistical mechanics is therefore adopted, and the diagrammatic technique for systems out of equilibrium is developed systematically, and a representation most appealing to physical intuition applied. Though most examples are taken from condensed matter physics, the book is intended to contribute to the cross-fertilization between all the fields of physics studying the influence of fluctuations, be they quantum or thermal or purely statistical, and to establish that the convenient technique to use is in fact that of non-equilibrium quantum field theory. The book should therefore be of interest to a wide audience of physicists; in particular the book is intended to be self-contained so that students of physics and physicists in general can benefit from its detailed expositions. It is even contended that the method is of importance for other fields such as chemistry, and of course useful for electrical engineers.

A complete allocation of the credit for the progress in developing and applying the real-time description of non-equilibrium states has not been attempted. However, the references, in particular the cited review articles, should make it possible for the interested reader to trace this information.

The book is intended to be sufficiently broad to serve as a text for a one- or two-semester graduate course on non-equilibrium statistical mechanics or condensed matter theory. It is also hoped that the book can serve as a useful reference book for courses on quantum field theory, physics of disordered systems, and quantum transport in general. It is hoped that this attempt to make the exposition as lucid as possible will be successful to the point that the book can be read by students with only elementary knowledge of quantum and statistical mechanics, and read with benefit on its own. Exercises have been provided in order to aid self-instruction.

I am grateful to Dr. Joachim Wabnig for providing figures.

Jørgen Rammer

Contents

1

Quantum fields

Quantum field theory is a necessary tool for the quantum mechanical description of processes that allow for transitions between states which differ in their particle content. Quantum field theory is thus quantum mechanics of an arbitrary number of particles. It is therefore mandatory for relativistic quantum theory since relativistic kinematics allows for creation and annihilation of particles in accordance with the formula for equivalence of energy and mass. Relativistic quantum theory is thus inherently dealing with many-body systems. One may, however, wonder why quantum field theoretic methods are so prevalent in condensed matter theory, which considers non-relativistic many-body systems. The reason is that, though not mandatory, it provides an efficient way of respecting the quantum statistics of the particles, i.e. the states of identical fermions or bosons must be antisymmetric and symmetric, respectively, under the interchange of pairs of identical particles. Furthermore, the treatment of spontaneously symmetry broken states, such as superfluids, is facilitated; not to mention critical phenomena in connection with phase transitions. Furthermore, the powerful functional methods of field theory, and methods such as the renormalization group, can by use of the non-equilibrium field theory technique be extended to treat non-equilibrium states and thereby transport phenomena.

It is useful to delve once into the underlying mathematical structure of quantum field theory, but the upshot of this chapter will be very simple: just as in quantum mechanics, where the transition operators, $|\phi\rangle\langle\psi|$, contain the whole content of quantum kinematics, and the *bra* and *ket* annihilate and create states in accordance with

$$(|\phi\rangle\langle\psi|)\,|\chi\rangle \;=\; \langle\psi|\chi\rangle\,|\phi\rangle \tag{1.1}$$

we shall find that in quantum field theory two types of operators do the same job. One of these operators, the creation operator, $a^\dagger$, is similar in nature to the *ket* in the transition operator, and the other, the annihilation operator, a, is similar to the action of the *bra* in Eq. (1.1), annihilating the state it operates on. Then the otherwise messy obedience of the quantum statistics of particles becomes a trivial matter expressed through the anti-commutation or commutation relations of the creation and annihilation operators.

1.1 Quantum mechanics

A short discussion of quantum mechanics is first given, setting the scene for the notation. In quantum mechanics, the state of a physical system is described by a vector, $|\psi\rangle$, providing a complete description of the system. The description is unique modulo a phase factor, i.e. the state of a physical system is properly represented by a ray, the equivalence class of vectors $e^{i\varphi}|\psi\rangle$, differing only by an overall phase factor of modulo one.

We consider first a single particle. Of particular intuitive importance are the states where the particle is definitely at a given spatial position, say $\mathbf{x}$, the corresponding state vector being denoted by $|\mathbf{x}\rangle$. The projection of an arbitrary state onto such a position state, the scalar product between the states,

$$\psi(\mathbf{x}) \;=\; \langle \mathbf{x}|\psi\rangle \;, \tag{1.2}$$

specifies the probability amplitude, the so-called wave function, whose absolute square is the probability for the event that the particle is located at the position in question.[1] The states of definite spatial positions are delta normalized

$$\langle \mathbf{x}|\mathbf{x}'\rangle \;=\; \delta(\mathbf{x}-\mathbf{x}') \;. \tag{1.3}$$

Of equal importance is the complementary representation in terms of the states of definite momentum, the corresponding state vectors denoted by $|\mathbf{p}\rangle$. Analogous to the position states they form a complete set or, equivalently, they provide a resolution of the identity operator, $\hat{I}$, in terms of the momentum state projection operators

$$\int d\mathbf{p}\; |\mathbf{p}\rangle\langle\mathbf{p}| \;=\; \hat{I} \;. \tag{1.4}$$

The appearance of an integral in Eq. (1.4) assumes space to be infinite, and the (conditional) probability amplitude for the event of the particle to be at position $\mathbf{x}$ *given* it has momentum $\mathbf{p}$ is specified by the plane wave function

$$\langle \mathbf{x}|\mathbf{p}\rangle \;=\; \frac{1}{(2\pi\hbar)^{3/2}}\, e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}} \;, \tag{1.5}$$

the transformation between the complementary representations being Fourier transformation. The states of definite momentum are therefore also delta normalized[2]

$$\langle \mathbf{p}|\mathbf{p}'\rangle \;=\; \delta(\mathbf{p}-\mathbf{p}') \;. \tag{1.6}$$

The possible physical momentum values are represented as eigenvalues, $\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle$, of the operator

$$\hat{\mathbf{p}} \;=\; \int d\mathbf{p}\; \mathbf{p}\, |\mathbf{p}\rangle\langle\mathbf{p}| \tag{1.7}$$

[1] Treating space as a continuum, the relevant quantity is of course the probability for the particle being in a small volume around the position in question, $P(\mathbf{x})\Delta\mathbf{x} = |\psi(\mathbf{x})|^2\Delta\mathbf{x}$, the absolute square of the wave function denoting a probability *density*.

[2] If the particle is confined in space, say confined in a box as often assumed, the momentum states are Kronecker normalized, $\langle \mathbf{p}|\mathbf{p}'\rangle = \delta_{\mathbf{p},\mathbf{p}'}$.

representing the physical quantity *momentum*. Similarly for the position of a particle. The average value of a physical quantity is thus specified by the matrix element of its corresponding operator, say the average position in state $|\psi\rangle$ is given by the three real numbers composing the vector $\langle\psi|\hat{\mathbf{x}}|\psi\rangle$. In physics it is customary to interpret a scalar product as the value of the *bra*, a linear functional on the state vector space, on the vector, *ket*, in question.[3]

The complementarity of the position and momentum descriptions is also expressed by the commutator, $[\hat{\mathbf{x}}, \hat{\mathbf{p}}] \equiv \hat{\mathbf{x}}\,\hat{\mathbf{p}} - \hat{\mathbf{p}}\,\hat{\mathbf{x}}$, of the operators representing the two physical quantities, being the c-number specified by the quantum of action

$$[\hat{\mathbf{x}}, \hat{\mathbf{p}}] \;=\; i\hbar\,. \tag{1.8}$$

The fundamental position and momentum representations refer only to the kinematical structure of quantum mechanics. The dynamics of a system is determined by the Hamiltonian $\hat{H} = H(\hat{\mathbf{p}}, \hat{\mathbf{x}})$, the operator specified according to the correspondence principle by Hamilton's function $H(\hat{\mathbf{p}}, \hat{\mathbf{x}})$, i.e. for a non-relativistic particle of mass m in a potential $V(\mathbf{x})$ the Hamiltonian, the energy operator, is

$$\hat{H} \;=\; \frac{\hat{\mathbf{p}}^2}{2m} \;+\; V(\hat{\mathbf{x}})\,. \tag{1.9}$$

It can often be convenient to employ the eigenstates of the Hamiltonian

$$\hat{H}\,|\epsilon_\lambda\rangle \;=\; \epsilon_\lambda\,|\epsilon_\lambda\rangle\,. \tag{1.10}$$

The completeness of the states of definite energy, $|\epsilon_\lambda\rangle$, is specified by *their* resolution of the identity

$$\sum_\lambda\, |\epsilon_\lambda\rangle\langle\epsilon_\lambda| = \hat{I} \tag{1.11}$$

here using a notation corresponding to the case of a discrete spectrum.

At each instant of time a complete description is provided by a state vector, $|\psi(t)\rangle$, thereby defining an operator, the time-evolution operator connecting state vectors at different times

$$|\psi(t)\rangle \;=\; \hat{U}(t,t')\,|\psi(t')\rangle\,. \tag{1.12}$$

Conservation of probability, conservation of the length of a state vector, or its normalized scalar product $\langle\psi(t)|\psi(t)\rangle = 1$, under time evolution, determines the evolution operator to be unitary, $U^{-1}(t,t') = U^\dagger(t,t')$. The dynamics is given by the Schrödinger equation

$$i\hbar\,\frac{d|\psi(t)\rangle}{dt} \;=\; \hat{H}\,|\psi(t)\rangle \tag{1.13}$$

and for an isolated system the evolution operator is thus the unitary operator

$$\hat{U}(t,t') \;=\; e^{-\frac{i}{\hbar}\hat{H}(t-t')}\,. \tag{1.14}$$

Here we have presented the operator calculus approach to quantum dynamics, the equivalent path integral approach is presented in Appendix A.

[3]For a detailed introduction to quantum mechanics we direct the reader to chapter 1 in reference [1].

In order to describe a physical problem we need to specify particulars, typically in the form of an initial condition. Such general initial condition problems can be solved through the introduction of the Green's function. The Green's function $G(\mathbf{x},t;\mathbf{x}',t')$ represents the solution to the Schrödinger equation for the particular initial condition where the particle is definitely at position $\mathbf{x}'$ at time t'

$$\lim_{t\searrow t'} \psi(\mathbf{x},t) \;=\; \delta(\mathbf{x}-\mathbf{x}') \;=\; \langle \mathbf{x},t'|\mathbf{x}',t'\rangle \;. \tag{1.15}$$

The solution of the Schrödinger equation corresponding to this initial condition therefore depends parametrically on $\mathbf{x}'$ (and t'), and is by definition the conditional probability density amplitude for the dynamics in question[4]

$$\psi_{\mathbf{x}',t'}(\mathbf{x},t) \;=\; \langle \mathbf{x},t|\mathbf{x}',t'\rangle \;=\; \langle \mathbf{x}|\hat{U}(t,t')|\mathbf{x}'\rangle \;\equiv\; G(\mathbf{x},t;\mathbf{x}',t') \;. \tag{1.16}$$

The Green's function, defined to be a solution of the Schrödinger equation, satisfies

$$\left(i\hbar\frac{\partial}{\partial t} \;-\; H(-i\hbar\nabla_{\mathbf{x}},\mathbf{x})\right) G(\mathbf{x},t;\mathbf{x}',t') = 0 \tag{1.17}$$

where, according to Eq. (1.3), the Hamiltonian in the position representation, H, is specified by the position matrix elements of the Hamiltonian

$$\langle \mathbf{x}|\hat{H}|\mathbf{x}'\rangle \;=\; H(-i\hbar\nabla_{\mathbf{x}},\mathbf{x})\;\delta(\mathbf{x}-\mathbf{x}') \;. \tag{1.18}$$

The Green's function, G, is the kernel of the Schrödinger equation on integral form (being a first order differential equation in time)

$$\psi(\mathbf{x},t) \;=\; \int d\mathbf{x}'\, G(\mathbf{x},t;\mathbf{x}',t')\,\psi(\mathbf{x}',t') \tag{1.19}$$

as identified in terms of the matrix elements of the evolution operator by using the resolution of the identity in terms of the position basis states

$$\langle \mathbf{x}|\psi(t)\rangle \;=\; \int d\mathbf{x}'\langle \mathbf{x}|\hat{U}(t,t')|\mathbf{x}'\rangle\langle \mathbf{x}'|\psi(t')\rangle \;. \tag{1.20}$$

The Green's function propagates the wave function, and we shall therefore also refer to the Green's function as the propagator. It completely specifies the quantum dynamics of the particle.

We note that the partition function of thermodynamics and the trace of the evolution operator are related by analytical continuation:

$$\begin{aligned} Z \;&=\; \mathrm{Tr}\, e^{-\hat{H}/kT} = \int d\mathbf{x}\;\langle \mathbf{x}|e^{-\hat{H}/kT}|\mathbf{x}\rangle \;=\; \mathrm{Tr}\,\hat{U}(-i\hbar/kT,0) \\ &=\; \int d\mathbf{x}\; G(\mathbf{x},-i\hbar/kT;\mathbf{x},0) \end{aligned} \tag{1.21}$$

[4] In the continuum limit the Green's function is not a normalizable solution of the Schrödinger equation, as is clear from Eq. (1.15).

showing that the partition function is obtained from the propagator at the imaginary time $\tau = -i\hbar/kT$. The formalisms of thermodynamics, i.e. equilibrium statistical mechanics, and quantum mechanics are thus equivalent, a fact we shall take advantage of throughout. The physical significance is the formal equivalence of quantum and thermal fluctuations.

Quantum mechanics can be formulated without the use of operators, viz. using Feynman's path integral formulation. In Appendix A, the path integral expressions for the propagator and partition function for a single particle are obtained. Various types of Green's functions and their properties for the case of a single particle are discussed in Appendix C, and their analytical properties are considered in Appendix D.

1.2 N-particle system

Next we consider a physical system consisting of N particles. If the particles in an assembly are distinguishable, i.e. different species of particles, an orthonormal basis in the N-particle state space $H^{(N)} = H_1 \otimes H_2 \otimes \cdots \otimes H_N$ is the (tensor) product states, for example specified in terms of the momentum quantum numbers of the particles

$$|\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N\rangle \equiv |\mathbf{p}_1\rangle \otimes |\mathbf{p}_2\rangle \otimes \cdots \otimes |\mathbf{p}_N\rangle \equiv |\mathbf{p}_1\rangle|\mathbf{p}_2\rangle \cdots |\mathbf{p}_N\rangle . \quad (1.22)$$

We follow the custom of suppressing the tensorial notation.

Formally everything in the following, where an N-particle system is considered, is equivalent no matter which complete set of single-particle states are used. In practice the choice follows from the context, and to be specific we shall mainly explicitly employ the momentum states, the choice convenient in practice for a spatially translational invariant system.[5] These states are eigenstates of the momentum operators

$$\hat{\mathbf{p}}_i \, |\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N\rangle = \mathbf{p}_i \, |\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N\rangle , \quad (1.23)$$

where tensorial notation for operators are suppressed, i.e.

$$\hat{\mathbf{p}}_i = \hat{I}_1 \otimes \cdots \hat{I}_{i-1} \otimes \hat{\mathbf{p}}_i \otimes \hat{I}_{i+1} \otimes \cdots \hat{I}_N , \quad (1.24)$$

each operating in the one-particle subspace dictated by its index. In particular the N-particle momentum states are eigenstates of the total momentum operator

$$\hat{\mathbf{P}}_N = \sum_{i=1}^{N} \hat{\mathbf{p}}_i \quad (1.25)$$

[5] In the next sections we shall mainly use the momentum basis, and refer in the following to the quantum numbers labeling the one-particle states as *momentum*, although any complete set of quantum numbers could equally well be used. The N-tuple $(\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N)$ is a complete description of the N-particle system if the particles do not posses internal degrees of freedom. In the following, where we for example have electrons in mind, we suppress for simplicity of notation the spin labeling and simply assume it is absorbed in the momentum labeling. If the particles have additional internal degrees of freedom, such as color and flavor, these are included in a similar fashion. If more than one type of species is to be considered simultaneously the species type, say quark and gluon, must also be indicated.