have true probabilities for the possible series of events, histories, emerging from the quantum description. In order to reconcile the probabilistic predictions of quantum mechanics with almost certainty to the deterministic predictions of classical mechanics, it is convenient to use a relaxed quantum logic.[87] In this way the certainty of implication becomes a quantitative question of probability: proposition α implies proposition β with a probability at most in error with the magnitude ϵ if $p(\beta;\alpha) \geq 1-\epsilon$. Having implication or to certainty limiting implication in our possession, we can reason about the probable course of events exhibited by an isolated system akin to how an experimenter goes about discussing an experiment or designing its equipment.[88] Sound reasoning about a quantum system has become a quantitative matter, a matter of calculation. The smaller the value of ϵ, the better will the reasoning and conclusions be in concordance with reality.

[87] For details on recovering classical physics we refer to the references [16] and [18].

[88] Extending the above analysis, we can conclude that particles keep on circulating in a storage ring in accordance with the classical equations of motion, because the probability for not doing so is by proper design insignificant.

Chapter 2

Diagrammatic Perturbation Theory

This chapter is concerned with propagators. After introducing the retarded and advanced propagator we study their perturbation theoretic structure in a potential in terms of diagrams. The scattering cross section is introduced, and the implications for the propagators of the discrete symmetries of space inversion and time reversal are established. The analytical properties of the propagators are discussed, and the spectral function introduced.

At present, the only general method available for gaining knowledge from the fundamental principles about the dynamics of a system is the perturbative study. This consists in dividing the Hamiltonian into one part representing a simpler well-understood problem and a nontrivial part, the effect of which is studied order by order. The expressions resulting from perturbation theory quickly become unwieldy. A convenient method of representing perturbative expressions by diagrams was invented by Feynman. Besides the appealing aspect of representing perturbative expressions by drawings, the diagrammatic method can also be used directly for reasoning and problem solving. The easily recognizable topology of diagrams makes the diagrammatic method a powerful tool for constructing approximation schemes as well as exact equations that may hold true beyond perturbation theory. Furthermore, by elevating the diagrams to be a representation of possible alternative physical processes, the diagrammatic representation becomes a suggestive tool providing physical intuition into quantum dynamics. We now embark on the construction of the diagrammatic representation starting from the canonical formalism presented in the first chapter.

2.1 Green's Functions and Propagators

The Schrödinger equation describing the dynamics of a single particle in the position representation is

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = H\psi(\mathbf{x},t)\,. \tag{2.1}$$

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'

$$\lim_{t \searrow t'} \psi(\mathbf{x}, t) \; = \; \delta(\mathbf{x} - \mathbf{x}') \; = <\mathbf{x}, t'|\mathbf{x}', t'> \; . \tag{2.2}$$

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[1]

$$\psi_{\mathbf{x}', t'}(\mathbf{x}, t) \; = \; K(\mathbf{x}, t; \mathbf{x}', t') \; \equiv \; G(\mathbf{x}, t; \mathbf{x}', t') \tag{2.3}$$

connecting the two incompatible complete descriptions defined by the operators $\hat{x}_H(t)$ and $\hat{x}_H(t')$.

The Green's function, being the kernel of the Schrödinger equation on integral form, eq.(1.5), specifies the dynamics of the system. We shall therefore refer to the Green's function as the propagator.[2] The propagator, being a transformation function, is the trace of the transition operator $\hat{P}(\mathbf{x}, t; \mathbf{x}', t')$[3]

$$G(\mathbf{x}, t; \mathbf{x}', t') \; = \; Tr(\hat{P}(\mathbf{x}, t; \mathbf{x}', t')) \; = \; Tr(|\mathbf{x}', t'><\mathbf{x}, t|) \; = \; <\mathbf{x}, t|\mathbf{x}', t'> \; . \tag{2.4}$$

Since the Green's function is defined to be a solution of the Schrödinger equation, we have (as also verified by differentiating eq.(2.4))

$$\{i\hbar\frac{\partial}{\partial t} - H\}G(\mathbf{x}, t; \mathbf{x}', t') = 0 \; . \tag{2.5}$$

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

$$\begin{aligned} Z \; &= \; Tr\, e^{-\hat{H}/kT} = \int d\mathbf{x} \; <\mathbf{x}|e^{-\hat{H}/kT}|\mathbf{x}> \; = \; Tr\, \hat{U}(-i\hbar/kT, 0) \\ &= \; \int d\mathbf{x} \; G(\mathbf{x}, -i\hbar/kT; \mathbf{x}, 0) \end{aligned} \tag{2.6}$$

showing that the partition function is obtained from the propagator at the imaginary time $\tau = -i\hbar/kT$.

[1]In the continuum limit the Green's function is not a normalizable solution of the Schrödinger equation as is clear from eq.(2.2).

[2]In appendix A the path integral expression for the propagator is derived starting from the transformation function.

[3]The absolute square of the propagator, the conditional probability density $P(\mathbf{x}, t\,; \mathbf{x}', t')$, can also be viewed as the probability density for a history since $P(\mathbf{x}, t\,; \mathbf{x}', t') \; = \; |G(\mathbf{x}, t; \mathbf{x}', t')|^2 \; = \; Tr(\hat{P}(\mathbf{x}, t)\hat{P}(\mathbf{x}', t'))$ is the probability for the history where the particle is at position $\mathbf{x}$ at time t given it was at position $\mathbf{x}'$ at time t'.

Exercise 2.1 *Derive for a particle in a potential the path integral expression for the imaginary-time propagator (consider the one-dimensional case for simplicity)*

$$\mathcal{G}(x, x', \hbar/kT) \; \equiv \; G(x, -i\hbar/kT; x', 0) = <x|e^{-\hat{H}/kT}|x'> = \int_{x(0)=x'}^{x(\hbar/kT)=x} \mathcal{D}x_\tau \;\, e^{-S_{\mathcal{E}}[x_\tau]/\hbar} \tag{2.7}$$

where the Euclidean action

$$S_{\mathcal{E}}[x_\tau] = \int_0^{\hbar/kT} d\tau \;\, L_{\mathcal{E}}(x_\tau, \dot{x}_\tau) \tag{2.8}$$

is specified in terms of the Euclidean Lagrange function

$$L_{\mathcal{E}}(x_\tau, \dot{x}_\tau) = \frac{1}{2}m\dot{x}_\tau^2 + V(x_\tau) \tag{2.9}$$

where the potential energy is "added" to the kinetic energy.

Solution

According to eq.(2.6) we obtain by writing $e^{-\hat{H}/kT}$ *as the product of* $N+1$ *identical operators* $e^{-\hat{H}/kT} = e^{-\hat{H}/(N+1)kT} \, .. \, e^{-\hat{H}/(N+1)kT}$*, and inserting* N *complete sets of states*

$$\begin{aligned} <x|e^{-\hat{H}/kT}|x'> \; &= \; \int dx_1 \int dx_2 .. \int dx_N \; <x|e^{-\hat{H}/NkT}|x_N><x_N|e^{-\hat{H}/NkT}|x_{N-1}> \\ &\quad \cdot \; <x_{N-1}|e^{-\hat{H}/NkT}|x_{N-2}> .. <x_1|e^{-\hat{H}/NkT}|x'> \; . \end{aligned} \tag{2.10}$$

We have introduced N *time slices in the so-called imaginary time interval* $[0, \hbar/kT]$*, each separated by the amount* $\Delta\tau = \hbar/(N+1)kT$*. The calculation is now analogous to the one of appendix A, eq.(A.3), except for the substitution* $i\Delta t \rightarrow \Delta\tau$*, and we obtain*

$$\begin{aligned} <x_n|e^{-\hat{H}/(N+1)kT}|x_{n-1}> \; &= \; <x_n|e^{-\frac{\Delta\tau}{\hbar}\hat{H}}|x_{n-1}> \\ &= \; \delta(x_n - x_{n-1}) - \frac{\Delta\tau}{\hbar} <x_n|\hat{H}|x_{n-1}> + \mathcal{O}(\Delta\tau^2). \\ &= \; \int\frac{dp_n}{2\pi\hbar} \, e^{\frac{i}{\hbar}p_n(x_n - x_{n-1}) - \frac{\Delta\tau}{\hbar}H(x_n, p_n)} + \mathcal{O}(\Delta\tau^2) \end{aligned} \tag{2.11}$$

where $H(x_n, p_n)$ *is Hamilton's function, eq.(A.6), and we get the path integral expression for the imaginary-time propagator*

$$\begin{aligned} <x|e^{-\hat{H}/kT}|x'> \; &= \; \lim_{N\to\infty} \int \prod_{n=1}^{N} dx_n \prod_{n=1}^{N+1} \frac{dp_n}{2\pi\hbar} \; e^{\frac{i}{\hbar}p_n(x_n - x_{n-1}) - \frac{\Delta\tau}{\hbar}H(x_n, p_n)} \\ &\equiv \; \int \frac{\mathcal{D}x_\tau \, \mathcal{D}p_\tau}{2\pi\hbar} \; e^{\frac{i}{\hbar}\int_0^{\hbar/kT} d\tau \; [p_\tau\dot{x}_\tau + iH(x_\tau, p_\tau)]} \end{aligned} \tag{2.12}$$

and upon performing the Gaussian momentum integrations the stated result (which is the expression in eq.(1.23) after a so-called Wick rotation, $it \to \tau = \hbar/kT$). Interpreting τ as a length, we note that the Euclidean Lagrange function $L_{\mathcal{E}}$ equals the potential energy of a string of "length" $L \equiv \hbar/kT$ and tension m, placed in the external potential V. The classical partition function for the string with ends fixed at x' and x is

$$Z_{cl}(x,x') \;=\; \int_{x(0)=x'}^{x(\hbar/kT)=x} \mathcal{D}x_\tau \; e^{-S_{\mathcal{E}}[x_\tau]/\hbar} \;=\; \mathcal{G}(x,\hbar/kT;x',0) \tag{2.13}$$

and we have established that the imaginary-time propagator is specified in terms of the classical partition function for the string. The propagator evaluated at imaginary time $-i\hbar/kT$, $G(x,-i\hbar/kT;x',0)$, equals the classical partition function $Z_{cl}(x,x')$ for a string of "length" $\hbar/kT$ evaluated at the "temperature" $1/\hbar$.

2.2 Retarded and Advanced Propagators

For later use we introduce the retarded Green's function or propagator (the choice of phase is for later convenience)

$$G^R(\mathbf{x},t;\mathbf{x}',t') \;\equiv\; \begin{cases} -iG(\mathbf{x},t;\mathbf{x}',t') & \text{for } t \geq t' \\ 0 & \text{for } t < t'\,. \end{cases} \tag{2.14}$$

The retarded propagator satisfies the equation

$$\{i\hbar\frac{\partial}{\partial t} - H\}G^R(\mathbf{x},t;\mathbf{x}',t') = \hbar\;\delta(\mathbf{x}-\mathbf{x}')\;\delta(t-t') \tag{2.15}$$

which in conjunction with the condition

$$G^R(\mathbf{x},t;\mathbf{x},t') \;=\; 0 \qquad \text{for} \quad t < t' \tag{2.16}$$

specifies the retarded propagator. The source term on the right-hand side of eq.(2.15) represents the discontinuity in the retarded propagator at time $t = t'$, and is recognized by integrating eq.(2.15) over an infinitesimal time interval around t'. The retarded Green's function propagates the wave function forward in time.[4]

According to eq.(2.4), the retarded propagator is given by

$$G^R(\mathbf{x},t;\mathbf{x}',t') \;=\; -i\theta(t-t')\; <\mathbf{x}|\hat{U}(t,t')|\mathbf{x}'> \tag{2.17}$$

[4]The retarded propagator also has the following interpretation: prior to time t' the particle is absent, and at time $t = t'$ the particle is created at point $\mathbf{x}'$, and is subsequently propagated according to the Schrödinger equation. In contrast to the relativistic quantum theory, this point of view of propagation is not mandatory in nonrelativistic quantum mechanics where the quantum numbers describing the particle species are conserved.

and is immediately seen to satisfy the initial condition

$$G^R(\mathbf{x},t'+0;\mathbf{x}',t') \;=\; -i\,\delta(\mathbf{x}-\mathbf{x}') \tag{2.18}$$

and due to the step function the condition eq.(2.16). By direct differentiation with respect to time it also immediately follows that the retarded propagator satisfies eq.(2.15).

We note the path integral expression for the retarded propagator (see also appendix A)

$$\begin{aligned} G^R(\mathbf{x},t;\mathbf{x}',t') \;&=\; -i\theta(t-t')G(\mathbf{x},t;\mathbf{x}',t') = -i\theta(t-t')K(\mathbf{x},t;\mathbf{x}',t') \\ &=\; -i\,\theta(t-t') \int_{\mathbf{x}_{t'}=\mathbf{x}'}^{\mathbf{x}_t=\mathbf{x}} \mathcal{D}\mathbf{x}_{\bar{t}}\; e^{\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\, L(\mathbf{x}_{\bar{t}},\dot{\mathbf{x}}_{\bar{t}})}\,. \end{aligned} \tag{2.19}$$

We shall also need the advanced propagator

$$G^A(\mathbf{x},t;\mathbf{x}',t') \;\equiv\; \begin{cases} 0 & \text{for } t > t' \\ iG(\mathbf{x},t;\mathbf{x}',t') & \text{for } t \leq t' \end{cases} \tag{2.20}$$

which propagates the wave function backwards in time, as we have for $t < t'$ for the wave function at time t

$$\psi(\mathbf{x},t) \;=\; -i\int d\mathbf{x}'\; G^A(\mathbf{x},t;\mathbf{x}',t')\,\psi(x',t') \tag{2.21}$$

in terms of the wave function at the later time t'.

The retarded and advanced propagators are related according to

$$G^A(\mathbf{x},t;\mathbf{x}',t') \;=\; [G^R(\mathbf{x}',t';\mathbf{x},t)]^*\,. \tag{2.22}$$

The advanced propagator is also a solution of eq.(2.15), but zero in the opposite time region as compared to the retarded propagator.

We note, that in the spatial representation we have

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') \;&=\; <\mathbf{x}|\hat{U}(t,t')|\mathbf{x}'> \;=\; i[G^R(\mathbf{x},t;\mathbf{x}',t') - G^A(\mathbf{x},t;\mathbf{x}',t')] \\ &\equiv\; A(\mathbf{x},t;\mathbf{x}',t') \end{aligned} \tag{2.23}$$

where we have introduced the notation A for the Green's function G, and also refer to it as the spectral function.

Introducing the retarded and advanced Green's operators

$$\hat{G}^R(t,t') \equiv -i\theta(t-t')\,\hat{U}(t,t')\;, \quad \hat{G}^A(t,t') \equiv i\theta(t'-t)\,\hat{U}(t,t') \tag{2.24}$$

we have for the evolution operator

$$\hat{U}(t,t') = i(\hat{G}^R(t,t') - \hat{G}^A(t,t')) \;\equiv\; \hat{G}(t,t') \;\equiv\; \hat{A}(t,t') \tag{2.25}$$

and the unitarity of the evolution operator is reflected in the hermitian relationship of the Green's operators

$$\hat{G}^A(t,t') = [\hat{G}^R(t',t)]^\dagger . \tag{2.26}$$

The retarded and advanced Green's operators are characterized as solutions to the same differential equation

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\hat{G}^{R(A)}(t,t') \;=\; \hbar\,\delta(t-t')\,\hat{I} \tag{2.27}$$

but are zero for different time relationship.

The various representations of the Green's operators are obtained by taking matrix elements. For example, in the momentum representation we have for the retarded propagator

$$G^R(\mathbf{p},t;\mathbf{p}',t') \;=\; -i\theta(t-t')<\mathbf{p},t|\mathbf{p}',t'> = <\mathbf{p}|\hat{G}^R(t,t')|\mathbf{p}'> . \tag{2.28}$$

Exercise 2.2 *Defining in general the imaginary-time propagator*

$$\mathcal{G}(\mathbf{x},\tau;\mathbf{x}',\tau') \;\equiv\; \theta(\tau-\tau')<\mathbf{x}|e^{-\frac{\hat{H}(\tau-\tau')}{\hbar}}|\mathbf{x}'> \tag{2.29}$$

show that for the Hamiltonian for a particle in a magnetic field

$$\hat{H} \;=\; \frac{1}{2m}\big(\hat{\mathbf{p}} - e\mathbf{A}(\hat{\mathbf{x}})\big)^2 \tag{2.30}$$

the imaginary-time propagator satisfies the equation

$$\left(\hbar\frac{\partial}{\partial\tau} + \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_{\mathbf{x}} - e\mathbf{A}(\mathbf{x})\right)^2\right)\mathcal{G}(\mathbf{x},\tau;\mathbf{x}',\tau') \;\equiv\; \hbar\,\delta(\mathbf{x}-\mathbf{x}')\,\delta(\tau-\tau') \tag{2.31}$$

and write down the path integral representation of the solution.

2.3 Free Particle Propagator

In the previous chapter we established, by appealing to correspondence, that the Hamiltonian for a (low-energy) free particle of mass m is Hamilton's function of the momentum operator

$$\hat{H}_0 \;=\; H_0(\hat{\mathbf{p}}) \;=\; \frac{\hat{\mathbf{p}}^2}{2m} . \tag{2.32}$$

The free particle propagator in the momentum representation

$$G_0^R(\mathbf{p},t;\mathbf{p}',t') \;=\; -i\theta(t-t')<\mathbf{p}|e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}|\mathbf{p}'> \tag{2.33}$$

is therefore given by

$$G_0^R(\mathbf{p},t;\mathbf{p}',t') \;=\; G_0^R(\mathbf{p},t,t')<\mathbf{p}|\mathbf{p}'> \;=\; G_0^R(\mathbf{p},t-t')\begin{cases}\delta(\mathbf{p}-\mathbf{p}')\\ \delta_{\mathbf{p},\mathbf{p}'}\end{cases} \tag{2.34}$$

where the Kronecker or delta function (depending on whether the particle is confined to a box or not) reflects the spatial translation invariance of free propagation. The compatibility of the energy and momentum of a free particle is reflected in the definite temporal oscillations of the propagator

$$G_0^R(\mathbf{p},t,t') \;=\; -i\theta(t-t')\,e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}(t-t')} \tag{2.35}$$

determined by the energy of the state in question

$$\epsilon_{\mathbf{p}} \;=\; \frac{\mathbf{p}^2}{2m} \tag{2.36}$$

the dispersion relation for a free particle.

Fourier transforming we obtain for the free particle propagator in the spatial representation

$$\begin{aligned} G_0^R(\mathbf{x},t;\mathbf{x}',t') \;&=\; -i\theta(t-t')<\mathbf{x}|e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}|\mathbf{x}'> \\ &=\; -i\theta(t-t')\left(\frac{m}{2\pi\hbar i(t-t')}\right)^{d/2} e^{\frac{im}{2\hbar}\frac{(\mathbf{x}-\mathbf{x}')^2}{t-t'}} \end{aligned} \tag{2.37}$$

in accordance with eq.(1.24).

Exercise 2.3 *Show that the retarded propagator in the momentum representation satisfies the equation*

$$\{i\hbar\frac{\partial}{\partial t} - \epsilon_{\mathbf{p}}\}\,G_0^R(\mathbf{p},t;\mathbf{p}',t') \;=\; i\hbar\,\delta(\mathbf{p}-\mathbf{p}')\,\delta(t-t') . \tag{2.38}$$

2.4 Perturbation Theory

Situations are ubiquitous where an interaction with a system is adequately described in terms of a time-dependent classical field. Furthermore, in perturbation theory we shall for calculational reasons encounter time-dependent Hamiltonians (though the Hamiltonian for a closed system is time independent). We therefore where the antitime-ordering symbol, $\tilde{T}$, orders the time sequence oppositely as compared to T, as the adjoint inverts the order of a sequence of operators.

Exercise 2.4 *Verify for an arbitrary operator $\hat{X}(t)$ the following property for time-ordered exponentials for the time relationship $t' < t'' < t$*

$$Te^{\int_{t'}^{t} d\bar{t}\,\hat{X}(\bar{t})} \;=\; Te^{\int_{t''}^{t} d\bar{t}\,\hat{X}(\bar{t})}\; Te^{\int_{t'}^{t''} d\bar{t}\,\hat{X}(\bar{t})} \,. \tag{2.50}$$

From the unitarity of the evolution operator, $\hat{I} = \hat{U}^\dagger(t,t')\,U(t,t')$, and eq.(2.48), one verifies readily (as also obtained by taking the adjoint of eq.(2.48)) that

$$-i\hbar\,\frac{\partial \hat{U}(t,t')^\dagger}{\partial t} = \hat{U}^\dagger(t,t')\,\hat{H}(t) \tag{2.51}$$

and using eq.(1.331) we get

$$-i\hbar\frac{\partial \hat{U}(t,t')}{\partial t'} = \hat{U}(t,t')\,\hat{H}(t') \tag{2.52}$$

thereby establishing that differentiating the time-ordered exponential, eq.(2.47), with respect to the lower integration limit brings down the Hamiltonian to the right with the time label given by the lower limit of the integral.

Exercise 2.5 *Consider a particle in the potential V (vanishing in the far past) for which we have the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$. Show that*

$$|\psi(t)> \;=\; |\phi(t)> + \frac{1}{i\hbar}\int_{-\infty}^{t} dt'\, e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\,\hat{V}(t')\,|\psi(t')> \tag{2.53}$$

is a solution of the Schrödinger equation provided $|\phi(t)>$ is a solution of the Schrödinger equation in the absence of the potential.

Solution

Upon Taylor-expanding the exponential to lowest or in Δt we obtain from eq.(2.53)

$$\frac{|\psi(t+\Delta t)> - |\psi(t)>}{\Delta t} - \frac{|\phi(t+\Delta t)> - |\phi(t)>}{\Delta t}$$

$$= \frac{1}{i\hbar\Delta t}\left(\int_{-\infty}^{t+\Delta t} dt'\, e^{-\frac{i}{\hbar}\hat{H}_0(t+\Delta t-t')}\,\hat{V}(t')\,|\psi(t')> - \int_{-\infty}^{t} dt'\, e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\,\hat{V}(t')\,|\psi(t')>\right)$$

$$= \frac{1}{\Delta t}\left(\frac{\Delta t}{i\hbar}\hat{H}_0 \int_{-\infty}^{t} dt'\, e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\,\hat{V}(t')\,|\psi(t')> + \Delta t\,\hat{V}(t)\,|\psi(t)>\right) \tag{2.54}$$

and thereby the sought result.

2.5 Interaction Picture

Let us consider a Hamiltonian consisting of two parts:

$$\hat{H}_t = \hat{H}_0 + \hat{H}'_t\,. \tag{2.55}$$

We can rewrite the evolution operator:

$$\hat{U}(t,t') \;=\; Te^{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\,\hat{H}_{\bar{t}}} \;=\; \hat{U}_0(t,t_r)\,\hat{U}_I(t,t')\,\hat{U}_0^\dagger(t',t_r) \tag{2.56}$$

in terms of the evolution operator in the so-called interaction picture, the Heisenberg picture with respect to $\hat{H}_0$,

$$\hat{U}_I(t,t') = Te^{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\,\hat{H}'_I(\bar{t})}\,. \tag{2.57}$$

An operator in the interaction picture is specified by[7]

$$\hat{H}'_I(t) \equiv \hat{U}_0^\dagger(t,t_r)\,\hat{H}'_t\,\hat{U}_0(t,t_r) \tag{2.58}$$

and assuming that $\hat{H}_0$ is time independent, we have for the evolution operator in the absence of $\hat{H}'_t$

$$\hat{U}_0^\dagger(t,t_r) = e^{\frac{i}{\hbar}\hat{H}_0(t-t_r)}\,. \tag{2.59}$$

The arbitrary reference time where the interaction and Schrödinger pictures coincide we denote by t_r.

We can derive the construction, eq.(2.56), explicitly, but let us here use our above derived differentiation rules, thereby noticing that the operators on the two sides of eq.(2.56) satisfy the same first-order differential equation, and are therefore identical as they satisfy the same initial condition.

Often it is convenient to take the reference time as zero, $t_r = 0$, and we have

$$Te^{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\,\hat{H}_{\bar{t}}} = e^{-\frac{i}{\hbar}\hat{H}_0 t}(Te^{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\,\hat{H}'_I(\bar{t})})e^{\frac{i}{\hbar}\hat{H}_0 t'} \tag{2.60}$$

where

$$\hat{H}'_I(t) \;=\; e^{\frac{i}{\hbar}\hat{H}_0 t}\,\hat{H}'_t\,e^{-\frac{i}{\hbar}\hat{H}_0 t}\,. \tag{2.61}$$

[7] We note, that had we studied the case where $\hat{H}'$ is time independent we would still encounter a time-dependent operator in the interaction picture, $\hat{H}'_I(t)$.

2.6 Propagation in a Potential

The simplest example of diagrammatic perturbation theory is the case of a particle in a scalar potential $V(\mathbf{x}, t)$; i.e., we consider the particle to be in an environment whose influence on the particle can be described in terms of a classical potential. We then have the Hamiltonian

$$\hat{H}_t = \hat{H}_p + \hat{V}_t \tag{2.62}$$

where the effect of the potential is represented by the operator

$$\hat{V}_t = V(\hat{\mathbf{x}}, t) \ . \tag{2.63}$$

The Hamiltonian in the absence of the potential, $\hat{H}_p$, we assume to be time independent.

The retarded propagator in the external potential is specified by the matrix element of the evolution operator

$$\begin{aligned} G^R(\mathbf{x}, t; \mathbf{x}', t') &= -i\theta(t - t') < \mathbf{x}|\hat{U}(t, t')|\mathbf{x}' > \\ &= -i\theta(t - t') <\mathbf{x}|T e^{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\, \hat{H}_{\bar{t}}}|\mathbf{x}'> \ . \end{aligned} \tag{2.64}$$

The perturbative expansion of the propagator is obtained by introducing the time-ordered exponential expressed in the interaction picture

$$T e^{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\, \hat{H}_{\bar{t}}} = \hat{U}_0(t, t_r)\, T e^{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\, V(\hat{\mathbf{x}}(\bar{t}), \bar{t})}\, \hat{U}_0^\dagger(t', t_r) \tag{2.65}$$

where we have used that the potential operator in the interaction picture is the potential function of the position operator in the interaction picture

$$\hat{V}_I(t) = \hat{U}_0^\dagger(t, t_r)\, V(\hat{\mathbf{x}}, t)\, \hat{U}_0(t, t_r) = V(\hat{\mathbf{x}}(t), t) \tag{2.66}$$

now dropping the index indicating the interaction picture as no confusion should arise

$$\hat{\mathbf{x}}(t) \equiv \hat{\mathbf{x}}_I(t) = \hat{U}_0^\dagger(t, t_r)\, \hat{\mathbf{x}}\, \hat{U}_0(t, t_r) \ . \tag{2.67}$$

Expanding the time-ordered exponential, we get the perturbative expansion of the propagator

$$\begin{aligned} G^R(\mathbf{x}, t; \mathbf{x}', t')) &= -i\theta(t - t') <\mathbf{x}, t|T \exp\{-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\hat{V}_I(\bar{t})\}|\mathbf{x}', t'> \\ &\equiv \sum_{n=0}^{\infty} G_n^R(\mathbf{x}, t; \mathbf{x}', t') \end{aligned} \tag{2.68}$$

where the n'th order term is equal to

$$\begin{aligned} G_n^R(\mathbf{x}, t; \mathbf{x}', t')) &= -i\theta(t - t')\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}\int_{t'}^{t}\prod_{m=1}^{n} dt_m <\mathbf{x}, t|T(V(\hat{\mathbf{x}}(t_n), t_n) \\ & V(\hat{\mathbf{x}}(t_{n-1}), t_{n-1}) .. V(\hat{\mathbf{x}}(t_2), t_2)\, V(\hat{\mathbf{x}}(t_1), t_1))\, |\mathbf{x}', t'> \end{aligned} \tag{2.69}$$

and the time-labeled states now denotes the eigenstates of the position operator in the interaction picture

$$\hat{\mathbf{x}}_I(t)\, |\mathbf{x}, t> = \mathbf{x}\, |\mathbf{x}, t> \ , \qquad |\mathbf{x}, t> = \hat{U}_0^{-1}(t, t_r)|\mathbf{x}> \ . \tag{2.70}$$

By inserting a complete set of such states

$$\hat{I} = \int d\mathbf{x}_i\, |\mathbf{x}_i, t_i><\mathbf{x}_i, t_i| \tag{2.71}$$

in front of each operator $\hat{V}_I(t_i) = V(\hat{\mathbf{x}}(t_i), t_i)$ in the perturbative expression, the operation of the potential operator is turned into multiplication by the value of the potential at the space-time point in question as

$$\begin{aligned} \hat{V}_I(t_i)|\mathbf{x}_i, t_i> &= V(\hat{\mathbf{x}}(t_i), t_i)|\mathbf{x}_i, t_i> = \left(\int d\mathbf{x}\, |\mathbf{x}, t_i>\, V(\mathbf{x}, t_i) <\mathbf{x}, t_i|\right)|\mathbf{x}_i, t_i> \\ &= V(\mathbf{x}_i, t_i)\, |\mathbf{x}_i, t_i> \ . \end{aligned} \tag{2.72}$$

The zeroth-order propagator, the propagator in the absence of the potential V, is given by

$$G_0^R(\mathbf{x}, t; \mathbf{x}', t') = -i\theta(t - t') <\mathbf{x}|e^{-\frac{i}{\hbar}\hat{H}_p(t-t')}|\mathbf{x}'> \ . \tag{2.73}$$

The first-order correction to the propagator is given by

$$G_1^R(\mathbf{x}, t; \mathbf{x}', t') = -\frac{1}{\hbar}\theta(t - t')\int_{t'}^{t} dt_1 <\mathbf{x}, t|V(\hat{\mathbf{x}}(t_1), t_1)|\mathbf{x}', t'> \ . \tag{2.74}$$

For the time relations $t \leq t_1 \leq t'$ we have for the step function

$$\theta(t - t') = \theta(t - t_1)\, \theta(t_1 - t') \tag{2.75}$$

and for the first-order term we therefore have the expression

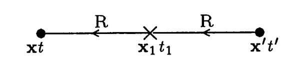
$$G_1^R(\mathbf{x}, t; \mathbf{x}', t') = \frac{1}{\hbar}\int d\mathbf{x}_1 \int_{-\infty}^{\infty} dt_1\, G_0^R(\mathbf{x}, t; \mathbf{x}_1, t_1)\, V(\mathbf{x}_1, t_1)\, G_0^R(\mathbf{x}_1, t_1; \mathbf{x}', t') \tag{2.76}$$

as the retarded propagators restrict the time integration to the original time interval.

The first-order contribution to the propagator can be thought of as a product of three terms: the amplitude for free particle propagation from space-time point $(\mathbf{x}', t')$ to $(\mathbf{x}_1, t_1)$, where the particle experiences interaction with the potential, described by the factor $V(\mathbf{x}_1, t_1)$, and finally the amplitude for free particle propagation from $(\mathbf{x}_1, t_1)$ to $(\mathbf{x}, t)$. Since the event of interaction with the potential, which we shall refer to as a scattering of the particle, can take place anywhere and at any time, we are summing over all these alternatives.

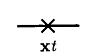
Graphically we represent the first-order term for the propagator by the diagram

$G_1^R(\mathbf{x}, t; \mathbf{x}', t') =$



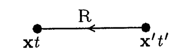
(2.77)

where a cross has been introduced to symbolize the interaction of the particle with the scalar potential



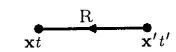
$$\equiv \frac{1}{\hbar} V(\mathbf{x}, t) \qquad (2.78)$$

and a thin line is used to represent the zeroth-order propagator



$$\equiv G_0^R(\mathbf{x}, t; \mathbf{x}', t') \qquad (2.79)$$

in order to distinguish it from the propagator in the presence of the potential V



$$\equiv G^R(\mathbf{x}, t; \mathbf{x}', t') \qquad (2.80)$$

depicted as a thick line. With this dictionary the analytical form, eq.(2.76), is obtained from the diagram, eq.(2.77), since integration is implied over the internal space-time point where interaction with the potential takes place.

Similarly we get for the second-order term by inserting complete sets of states

$$\begin{aligned} G_2^R(\mathbf{x}, t; \mathbf{x}', t') &= -i\theta(t - t') \left(\frac{-i}{\hbar}\right)^2 \int_{t'}^{t} dt_2 \int_{t'}^{t_2} dt_1 <\mathbf{x}, t|\mathbf{x}_2, t_2> V(\mathbf{x}_2, t_2) \\ & \quad <\mathbf{x}_2, t_2|\mathbf{x}_1, t_1> V(\mathbf{x}_1, t_1) <\mathbf{x}_1, t_1|\mathbf{x}', t'> \\ &= \hbar^{-2} \int d\mathbf{x}_2 \int_{-\infty}^{\infty} dt_2 \int d\mathbf{x}_1 \int_{-\infty}^{\infty} dt_1 G_0^R(\mathbf{x}, t; \mathbf{x}_2, t_2) V(\mathbf{x}_2, t_2) G_0^R(\mathbf{x}_2, t_2; \mathbf{x}_1, t_1) \\ & \quad V(\mathbf{x}_1, t_1) G_0^R(\mathbf{x}_1, t_1; \mathbf{x}', t') \end{aligned} \qquad (2.81)$$

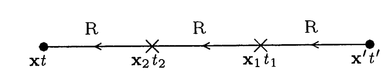
where we in the last equality have utilized that for the time relationship, $t' \leq t_1 \leq t_2 \leq t$, we have for the step function

$$\theta(t - t') = \theta(t - t_2)\, \theta(t_2 - t_1)\, \theta(t_1 - t') \qquad (2.82)$$

and we can lift the time integration limitations as the step functions automatically limit the integration region to the original one.

The second-order term for the propagator is therefore represented diagrammatically by

$$G_2^R(\mathbf{x}, t; \mathbf{x}', t') =$$



(2.83)

corresponding to propagation governed by $\hat{H}_p$ in between the scattering twice by the potential.

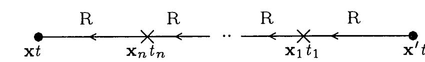
Repeating this scheme of inserting complete sets of states, letting the system propagate through all the possible position property values at all possible times,

we obtain that the n'th order term consists of n scatterings by the potential and $n + 1$ propagators

$$\begin{aligned} G_n^R(\mathbf{x}, t; \mathbf{x}', t') &= \frac{1}{\hbar^n} \int \prod_{m=1}^{n} d\mathbf{x}_m \int_{t'}^{t} \prod_{m=1}^{n} dt_m\, V(\mathbf{x}_n) V(\mathbf{x}_{n-1}) \,..\, V(\mathbf{x}_2) V(\mathbf{x}_1) \\ & \quad G_0^R(\mathbf{x}, t; \mathbf{x}_n, t_n)\, G_0^R(\mathbf{x}_n, t_n; \mathbf{x}_{n-1}, t_{n-1}) \,..\, G_0^R(\mathbf{x}_1, t_1; \tilde{\mathbf{x}}, t') \end{aligned} \qquad (2.84)$$

represented diagrammatically by

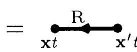
$$G_n^R(\mathbf{x}, t; \mathbf{x}', t') =$$

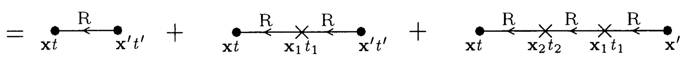


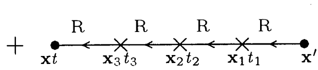
(2.85)

and the perturbative expression for the exact propagator is represented by the infinite sum of terms

$$G^R(\mathbf{x}, t; \mathbf{x}', t') =$$



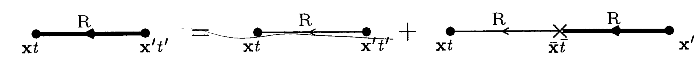




(2.86)

Following Feynman we can elevate the diagrams to represent alternative physical scattering processes. The propagator in a potential being the sum of all possible scattering alternatives for the particle: not being scattered, being scattered once, being scattered twice, etc.

Such a series of scattering processes where each subsequent process has an extra scattering event and propagator (each subsequent diagram has an extra cross and propagator line) is iterative, and the propagator for the particle in a potential satisfies the diagrammatic equation



(2.87)

as seen by iteration. Analytically we have the equation

$$G^R(\mathbf{x}, t; \mathbf{x}', t') = G_0^R(\mathbf{x}, t; \mathbf{x}', t') + \frac{1}{\hbar} \int d\bar{\mathbf{x}} \int_{-\infty}^{\infty} d\bar{t}\, G_0^R(\mathbf{x}, t; \bar{\mathbf{x}}, \bar{t}) V(\bar{\mathbf{x}}, \bar{t}) G^R(\bar{\mathbf{x}}, \bar{t}; \mathbf{x}', t') \,. \qquad (2.88)$$

The equation for the advanced propagator we obtain by using its relationship to the retarded propagator, eq.(2.22),

$$G^A(\mathbf{x},t;\mathbf{x}',t') \;=\; G_0^A(\mathbf{x},t;\mathbf{x}',t') \;+\; \frac{1}{\hbar}\int\! d\bar{\mathbf{x}}\int_{-\infty}^{\infty}\! d\bar{t}\; G^A(\mathbf{x},t;\bar{\mathbf{x}},\bar{t})V(\bar{\mathbf{x}},\bar{t})G_0^A(\bar{\mathbf{x}},\bar{t};\mathbf{x}',t') \tag{2.89}$$

or diagrammatically

(2.90)

with a convention for drawing the diagrams for the advanced propagator that makes explicit the backwards-in-time propagation.

Exercise 2.6 *Derive the perturbation expansion from the path integral formalism.*

Solution

From eq.(1.23) we obtain

$$K(\mathbf{x},t;\mathbf{x}',t') \;=\; \int_{\mathbf{x}_{t'}=\mathbf{x}'}^{\mathbf{x}_t=\mathbf{x}} \mathcal{D}\mathbf{x}_{\bar{t}}\; e^{\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,\frac{1}{2}m\dot{\mathbf{x}}_{\bar{t}}^2}\; e^{-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,V(\mathbf{x}_{\bar{t}},\bar{t})}$$

$$= \int_{\mathbf{x}_{t'}=\mathbf{x}'}^{\mathbf{x}_t=\mathbf{x}} \mathcal{D}\mathbf{x}_{\bar{t}}\; e^{\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,\frac{1}{2}m\dot{\mathbf{x}}_{\bar{t}}^2}\left(1 \;+\; \frac{-i}{\hbar}\int_{t'}^{t}dt_1\; V(\mathbf{x}_{t_1},t_1)\right.$$

$$\left. +\; \frac{1}{2!}\left(\frac{-i}{\hbar}\right)^2\int_{t'}^{t}dt_2\int_{t'}^{t}dt_1\; V(\mathbf{x}_{t_2},t_2)\,V(\mathbf{x}_{t_1},t_1) \;+\; \ldots\right)\,. \tag{2.91}$$

Consider the first-order term. In the discretized form of the path integral we choose one of the intermediate times as the one dictated by the integration over t_1. There are N_1 and N_2 other internal moments of time, before and after the one singled out, respectively. The corresponding internal spatial integrations, and the number of "measure"-factors produces the product of the free propagators $K_0(\mathbf{x}_1,t_1;\mathbf{x}',t')$ and $K_0(\mathbf{x},t;\mathbf{x}_1,t_1)$, and we obtain for the first-order correction to the propagator

$$K_1(\mathbf{x},t;\mathbf{x}',t') \;=\; \frac{-i}{\hbar}\int_{t'}^{t}dt_1\int\! d\mathbf{x}_1\; K_0(\mathbf{x},t;\mathbf{x}_1,t_1)\,V(\mathbf{x}_{t_1},t_1)\,K_0(\mathbf{x}_1,t_1;\mathbf{x}',t')\,. \tag{2.92}$$

In the second-order term we choose t_1 and t_2 as intermediate times. Since this can be done in two ways, $t_1 < t_2$ or $t_1 > t_2$, giving identical contributions and thereby canceling the factor $1/2!$, we obtain the expression in eq.(2.81). Similarly for the higher order terms, and we reproduce the perturbation series depicted diagrammatically in eq.(2.86).

2.6.1 Momentum Representation

For calculational purposes the momentum representation is often useful. In the momentum representation we encounter all the same manipulations as we did in the position representation except that we have **p**'s instead of **x**'s, and we have for the retarded propagator in the momentum representation

$$G^R(\mathbf{p},t;\mathbf{p}',t') = -i\theta(t-t') < \mathbf{p},t|\mathbf{p}',t' > = -i\theta(t-t') < \mathbf{p}|Te^{-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,\hat{H}_{\bar{t}}}|\mathbf{p}' > \,. \tag{2.93}$$

For the n'th order term in the perturbative expansion of the propagator

$$G^R(\mathbf{p},t;\mathbf{p}',t') = \sum_{n=0}^{\infty} G_n^R(\mathbf{p},t;\mathbf{p}',t') \tag{2.94}$$

we have

$$G_n^R(\mathbf{p},t;\mathbf{p}',t') = -i\theta(t-t')\frac{\left(\frac{-i}{\hbar}\right)^n}{n!}\int_{t'}^{t}\prod_{m=1}^{n}dt_m < \mathbf{p},t|T(\hat{V}_I(t_n)\hat{V}_I(t_{n-1})..\hat{V}_I(t_1))|\mathbf{p}',t'> \tag{2.95}$$

where the interaction picture momentum eigenstates

$$\hat{\mathbf{p}}_I(t)\,|\mathbf{p},t> = \mathbf{p}\,|\mathbf{p},t> \tag{2.96}$$

has been introduced.[8]

For the propagator in the absence of the potential V we have

$$G_0^R(\mathbf{p},t;\mathbf{p}',t') \;=\; -i\theta(t-t')\,<\mathbf{p}|e^{-\frac{i}{\hbar}\hat{H}_p(t-t')}|\mathbf{p}'> \,. \tag{2.97}$$

In order to calculate the propagator to first order, we insert complete sets of momentum eigenstates and obtain

$$G_1^R(\mathbf{p},t;\mathbf{p}',t') = \frac{1}{\hbar}\int_{-\infty}^{\infty}dt_1\int_{\mathbf{p}_1',\mathbf{p}_1} G_0^R(\mathbf{p},t;\mathbf{p}_1,t_1) < \mathbf{p}_1,t_1|\hat{V}_I(t_1)|\mathbf{p}_1',t_1> G_0^R(\mathbf{p}_1',t_1;\mathbf{p}',t') \tag{2.98}$$

where the interaction with the potential in the momentum representation is specified by (in three spatial dimensions)

$$<\mathbf{p},t|\hat{V}_I(t)|\mathbf{p}',t> \;=\; <\mathbf{p}|\hat{V}_t|\mathbf{p}'> \;=\; \begin{cases} (2\pi\hbar)^{-3}\int d\mathbf{x}\, e^{-\frac{i}{\hbar}\mathbf{x}\cdot(\mathbf{p}-\mathbf{p}')}\; V(\mathbf{x},t) \\ V^{-1}\int_V d\mathbf{x}\, e^{-\frac{i}{\hbar}\mathbf{x}\cdot(\mathbf{p}-\mathbf{p}')}\, V(\mathbf{x},t) \end{cases} \tag{2.99}$$

[8] We suppress the index distinguishing these states from the states in eq.(2.93) defined by the momentum operator in the Heisenberg picture as it is clear from the context which states are involved.

depending on whether we have a particle in a box of volume V (exceeding the range of the potential), or in infinite space[9]

$$<\mathbf{x},t|\mathbf{p},t> \;=\; <\mathbf{x}|\mathbf{p}> \;=\; \begin{cases} (2\pi\hbar)^{-3/2} e^{\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{p}} \\ \\ V^{-1/2} e^{\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{p}} \end{cases} \tag{2.100}$$

and we have in eq.(2.98) introduced the context-dependent notation

$$\sum_{\mathbf{p}} \;\leftrightarrow\; \int_{\mathbf{p}} \;\leftrightarrow\; \int_{-\infty}^{\infty} \!\! d\mathbf{p} \;. \tag{2.101}$$

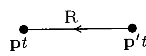
In the momentum representation we therefore have the same first-order diagram as in the spatial representation

$$G_1^R(\mathbf{p},t;\mathbf{p}',t') \;=$$ 

(2.102)

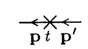
however, with the momentum representation interpretation of the diagram: The propagator between momentum values $\mathbf{p}'$ and $\mathbf{p}$ in the absence of the potential V we represent diagrammatically by a thin line[10]

$$G_0^R(\mathbf{p},t;\mathbf{p}',t') \;=\; -i\theta(t-t') < \mathbf{p}| e^{-\frac{i}{\hbar}\hat{H}_p(t-t')}|\mathbf{p}' >$$

$$\equiv$$ 

(2.103)

and in the momentum representation the cross designates the matrix element



$$=\; \frac{1}{\hbar} < \mathbf{p}|\hat{V}_t|\mathbf{p}'> \tag{2.104}$$

and signifies the momentum change due to the scattering by the potential. Summation (integration) over all alternative intermediate momenta, and integration over time is implied according to eq.(2.98).

For the second-order term we similarly obtain from eq.(2.95)

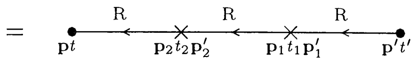
$$G_2^R(\mathbf{p},t;\mathbf{p}',t') \;=\; \frac{1}{\hbar^2}\int_{-\infty}^{\infty}\!\! dt_2 \!\int_{-\infty}^{\infty}\!\! dt_1 \int_{\mathbf{p}_1,\mathbf{p}'_1,\mathbf{p}_2,\mathbf{p}'_2} G_0^R(\mathbf{p},t;\mathbf{p}_2,t_2) < \mathbf{p}_2|\hat{V}_{t_2}|\mathbf{p}'_2 >$$

$$G_0^R(\mathbf{p}'_2,t_2;\mathbf{p}_1,t_1) < \mathbf{p}_1|\hat{V}_{t_1}|\mathbf{p}'_1 > G_0^R(\mathbf{p}'_1,t_1;\mathbf{p}',t') \tag{2.105}$$

[9] We shall often interchange between the notation for a particle in a finite volume V (with appropriately imposed boundary conditions), and the continuum notation.

[10] The propagator is in the absence of the potential V invariant with respect to displacements in time as $\hat{H}_p$ was assumed time independent, a constraint we could easily relax.

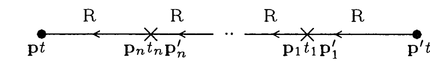
and diagrammatically

$$G_2^R(\mathbf{p},t;\mathbf{p}',t') \;=$$ 

(2.106)

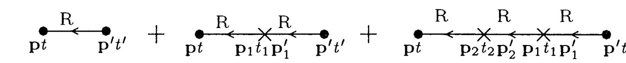
corresponding to propagation according to the Hamiltonian $\hat{H}_p$ in between the scattering by the potential where the momentum of the particle is changed.

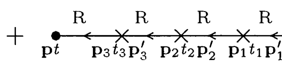
Repeating the scheme of inserting complete sets of momentum eigenstates we obtain that the n'th order term consists of n scatterings by the potential and $n+1$ propagators

$$G_n^R(\mathbf{p},t;\mathbf{p}',t') \;=$$ 

(2.107)

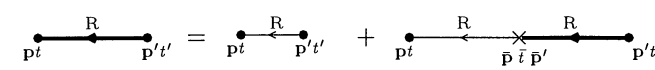
and the exact propagator is represented by the infinite set of diagrams

$$G^R(\mathbf{p},t;\mathbf{p}',t') \;=$$ 

$+$ 

$+ \;\ldots\;.$ (2.108)

The propagator in the momentum representation for a particle in a potential is therefore by iteration seen to satisfy the diagrammatic equation

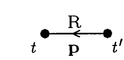


(2.109)

and analytically the equation

$$G^R(\mathbf{p},t;\mathbf{p}',t') = G_0^R(\mathbf{p},t;\mathbf{p}',t') + \frac{1}{\hbar}\int_{\bar{\mathbf{p}},\bar{\mathbf{p}}'}\int_{-\infty}^{\infty}\!\! d\bar{t}\, G_0^R(\mathbf{p},t;\bar{\mathbf{p}},\bar{t}) < \bar{\mathbf{p}}|\hat{V}_{\bar{t}}|\bar{\mathbf{p}}'> G^R(\bar{\mathbf{p}}',\bar{t};\mathbf{p}',t')\,. \tag{2.110}$$

In the case where the particle Hamiltonian, $\hat{H}_p$, represents a free particle, the zeroth-order propagator is the free propagator, eq.(2.33), and we introduce the diagrammatic representation for the amplitude for free propagation in momentum state $\mathbf{p}$, eq.(2.35),

$$G_0^R(\mathbf{p},t,t') \;=$$ 

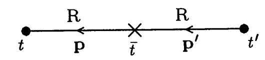
$$=\; -i\theta(t-t')\, e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}(t-t')}\,. \tag{2.111}$$

The first-order correction to the propagator due to the potential, eq.(2.98), reduces in this case to

$$G_1^R(\mathbf{p},t;\mathbf{p}',t') = \frac{1}{\hbar}\int_{-\infty}^{\infty} d\bar{t}\, G_0^R(\mathbf{p},t,\bar{t}) < \mathbf{p}|\hat{V}_{\bar{t}}|\mathbf{p}'> G_0^R(\mathbf{p}',\bar{t},t') \qquad (2.112)$$

corresponding diagrammatically to

$$G_1^R(\mathbf{p},t;\mathbf{p}',t') \quad = \qquad (2.113)$$



Similarly we get to second order in the potential

$$G_2^R(\mathbf{p},t;\mathbf{p}',t') = \frac{1}{\hbar^2}\int_{\mathbf{p}''}\int_{-\infty}^{\infty}dt_2\int_{-\infty}^{\infty}dt_1\; G_0^R(\mathbf{p},t,t_2) < \mathbf{p}|\hat{V}_{t_2}|\mathbf{p}''> G_0^R(\mathbf{p}'',t_2,t_1)$$
$$< \mathbf{p}''|\hat{V}_{t_1}|\mathbf{p}'> G_0^R(\mathbf{p}',t_1,t')$$

$$= \qquad (2.114)$$

and the momentum representation of the propagator in the potential is obtained by iterating the following equation

$$\qquad (2.115)$$

Analytically we have the equation

$$G^R(\mathbf{p},t;\mathbf{p}',t') = G_0^R(\mathbf{p},t;\mathbf{p}',t') + \frac{1}{\hbar}\int_{\mathbf{p}''}\int d\bar{t}\, G_0^R(\mathbf{p},t,\bar{t}) < \mathbf{p}|\hat{V}_{\bar{t}}|\mathbf{p}''> G^R(\mathbf{p}'',\bar{t};\mathbf{p}',t') . \qquad (2.116)$$

2.6.2 Propagation in a Static Potential

In the case the system is isolated, the potential is time independent

$$\hat{H} = \hat{H}_p + V(\hat{\mathbf{x}}) \qquad (2.117)$$

and the propagator only depends on the time difference. In the momentum representation, for example, we then have for the propagator

$$G^R(\mathbf{p},t;\mathbf{p}',t') = G^R(\mathbf{p},\mathbf{p}';t-t') = < \mathbf{p},t|\mathbf{p}',t' >$$
$$= < \mathbf{p}|e^{-\frac{i}{\hbar}\hat{H}(t-t')}|\mathbf{p}'> . \qquad (2.118)$$

We therefore Fourier transform with respect to time[11]

$$G^R(\mathbf{p},\mathbf{p}',E) \equiv \frac{1}{\hbar}\int_{-\infty}^{\infty} d(t-t')\; e^{\frac{i}{\hbar}(E+i0)(t-t')}\, G^R(\mathbf{p},t;\mathbf{p}',t') \qquad (2.119)$$

and for the inverse transform we have

$$G^R(\mathbf{p},\mathbf{p}',t-t') = \frac{1}{2\pi}\int_{-\infty+i0}^{\infty+i0} dE\; e^{-\frac{i}{\hbar}E(t-t')}\, G^R(\mathbf{p},\mathbf{p}',E) . \qquad (2.120)$$

We shall call E the energy variable, emphasizing that the above Fourier transformation is not between property representations.

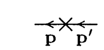
The invariance with respect to displacements in time is transparently reflected on a term-by-term basis in the perturbation expansion. In order to be specific let us assume that the particle is free in the absence of the potential V. The momentum representation and energy representations are then identical, and the free propagator in the momentum representation is just an oscillating exponential function of time, eq.(2.111).[12] The time convolutions of propagators in the perturbative expansion will then by Fourier transformation with respect to time be turned into simple products of Fourier-transformed propagators. The propagators will all have the same energy variable, reflecting the energy conservation in elastic scattering.

From the first-order term, eq.(2.112), we obtain by Fourier transformation

$$G_1^R(\mathbf{p},\mathbf{p}',E) = G_0^R(\mathbf{p},E) < \mathbf{p}|\hat{V}|\mathbf{p}'> G_0^R(\mathbf{p}',E) \qquad (2.121)$$

as for a static potential we have

$$< \mathbf{p},t|\hat{V}_I(t)|\mathbf{p}',t> = < \mathbf{p}|\hat{V}|\mathbf{p}'> = \qquad (2.122)$$



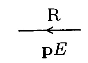
and we now represent this matrix element by a cross. The Fourier transform with respect to time of the free propagator, eq.(2.35), is given by

$$G_0^R(\mathbf{p},E) = \frac{1}{E-\epsilon_{\mathbf{p}}+i0} \qquad (2.123)$$

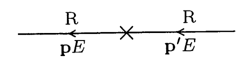
[11] We observe that the retarded propagator is analytic in the upper half plane. The discussion of the analytic properties of propagators being deferred to the following section.

[12] It is of course not essential for exploiting the invariance with respect to displacements in time, that the particle in the absence of the potential V is assumed otherwise free. The particle could, for example, be exposed to a time-independent magnetic field. In that case, we would then just have to use the energy-representation specified by the eigenstates of the particle Hamiltonian $\hat{H}_p$ for which the propagator oscillates in time according to the energy value in question.

for which we introduce the diagrammatic notation

$$G_0^R(\mathbf{p}, E) \;\equiv$$  . (2.124)

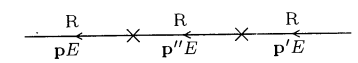
The first-order correction to the propagator is then specified diagrammatically by

$$G_1^R(\mathbf{p}, \mathbf{p}', E) \;=$$  . (2.125)

Similarly, by Fourier transforming eq.(2.35) with respect to time, we get for the second-order term

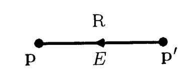
$$G_2^R(\mathbf{p}, \mathbf{p}', E) \;=\; G_0^R(\mathbf{p}, E) \left(\sum_{\mathbf{p}''} <\mathbf{p}|\hat{V}|\mathbf{p}''> G_0^R(\mathbf{p}'', E) <\mathbf{p}''|\hat{V}|\mathbf{p}'> \right) G_0^R(\mathbf{p}', E) \tag{2.126}$$

and diagrammatically

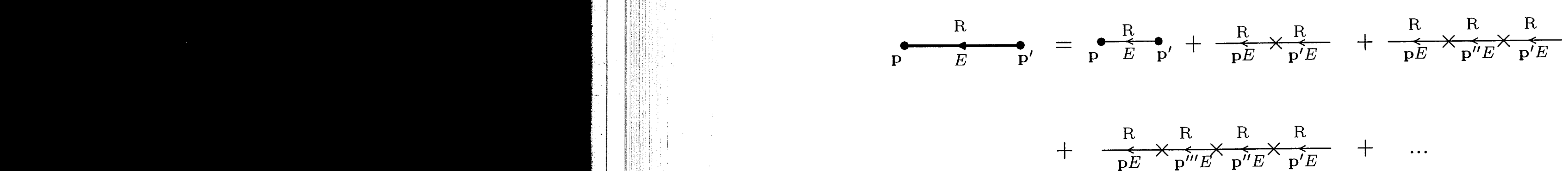
$$G_2^R(\mathbf{p}, \mathbf{p}', E) \;=$$  (2.127)

where a summation over all the possible alternative intermediate momentum values $\mathbf{p}''$ is implied.

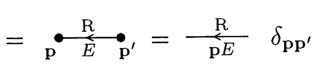
For the propagator in a static potential

$$G^R(\mathbf{p}, \mathbf{p}', E) \;\equiv$$  (2.128)

we then obtain the diagrammatic representation

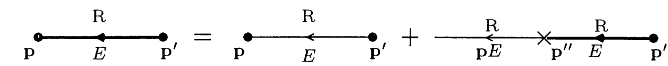
 (2.129)

where we have introduced the diagrammatic notation

$$G_0^R(\mathbf{p}, \mathbf{p}', E) \;=\; G_0^R(\mathbf{p}, E)\, \delta_{\mathbf{p}\mathbf{p}'} \;=$$  $\delta_{\mathbf{p}\mathbf{p}'}$ (2.130)

in order to absorb the Kronecker function in the free propagation term.

The full propagator is obtained by iterating the equation

 (2.131)

which analytically takes the form

$$\begin{aligned} G^R(\mathbf{p}, \mathbf{p}', E) &= G_0^R(\mathbf{p}, \mathbf{p}', E) + G_0^R(\mathbf{p}, E) \sum_{\mathbf{p}''} <\mathbf{p}|\hat{V}|\mathbf{p}''> G^R(\mathbf{p}'', \mathbf{p}', E) \\ &= G_0^R(\mathbf{p}, \mathbf{p}', E) \,+\, G_0^R(\mathbf{p}, E) \frac{1}{V} \sum_{\mathbf{p}''} V(\mathbf{p} - \mathbf{p}'') G^R(\mathbf{p}'', \mathbf{p}', E) \end{aligned} \tag{2.132}$$

where we have introduced the Fourier transform of the potential

$$V(\mathbf{p}) \;\equiv\; V <\mathbf{p}|\hat{V}|\mathbf{0}> = \int_V d\mathbf{x}\; e^{-\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{p}}\, V(\mathbf{x}) \tag{2.133}$$

for the case of a particle confined to a volume of size V.

2.7 Analytic Properties of Green's Functions

For an isolated system, where the Hamiltonian is time independent, we can for any complex number E with a positive imaginary part, transform the retarded Green's operator, eq.(2.24), according to

$$\hat{G}_E^R \;=\; \frac{1}{\hbar} \int_{-\infty}^{\infty} d(t - t')\; e^{\frac{i}{\hbar}E(t-t')}\, \hat{G}^R(t - t') \,. \tag{2.134}$$

The Fourier transform is obtained as the analytic continuation from the upper half plane, $\Im m E > 0$. According to eq.(2.27) we have for $\Im m E > 0$ the equation

$$\left(E - \hat{H}\right) \hat{G}_E^R \;=\; \hat{I} \,. \tag{2.135}$$

Analogously we obtain that the advanced Green's operator is the solution of the same equation

$$\left(E - \hat{H}\right) \hat{G}_E \;=\; \hat{I} \tag{2.136}$$

for values of the energy variable E in the lower half-plane, $\Im m E < 0$, and by analytical continuation to the real axis

$$\hat{G}_E^A \;\equiv\; \frac{1}{\hbar} \int_{-\infty}^{\infty} dt\; e^{\frac{i}{\hbar}Et}\, \hat{G}^A(t) \,. \tag{2.137}$$

We note the Fourier inversion formulas

$$\hat{G}^{R(A)}(t) = \frac{1}{2\pi} \int_{-\infty \,(\stackrel{+}{-})\, i0}^{\infty \,(\stackrel{+}{-})\, i0} dE\; e^{-\frac{i}{\hbar}Et}\, \hat{G}_E^{R(A)} \tag{2.138}$$

and the hermitian property, eq.(2.26), leads to the relationship

$$\hat{G}_E^A = [\hat{G}_{E^*}^R]^\dagger \,. \tag{2.139}$$

We introduce the Green's operator

$$\hat{G}_E \equiv \begin{cases} \hat{G}^R_E & \text{for } \Im m E > 0 \\ \hat{G}^A_E & \text{for } \Im m E < 0 \end{cases} \tag{2.140}$$

for which we have the spectral representation

$$\hat{G}_E = \frac{1}{E - \hat{H}} = \sum_\lambda \frac{|\epsilon_\lambda><\epsilon_\lambda|}{E - \epsilon_\lambda} \tag{2.141}$$

where $|\epsilon_\lambda>$ is the eigenstates of the Hamiltonian

$$\hat{H}\,|\epsilon_\lambda> = \epsilon_\lambda\,|\epsilon_\lambda> \ . \tag{2.142}$$

The analytic properties of the retarded and advanced Green's operators leads, by an application of Cauchy's theorem, to the spectral representations

$$\hat{G}^{R(A)}_E = \int_{-\infty}^{\infty} \frac{dE'}{2\pi} \frac{\hat{A}_{E'}}{E - E' \overset{+}{(-)} i0} \tag{2.143}$$

where we have introduced the spectral operator, the discontinuity of the Green's operator across the real axis

$$\begin{aligned} \hat{A}_E &\equiv i(\hat{G}^R_E - \hat{G}^A_E) = i(\hat{G}_{E+i0} - \hat{G}_{E-i0}) \\ &= 2\pi\,\delta(E - \hat{H}) = 2\pi \sum_\lambda |\epsilon_\lambda><\epsilon_\lambda|\,\delta(E - \epsilon_\lambda) \ . \end{aligned} \tag{2.144}$$

Equivalently, we have the relationship between real and imaginary parts of, say, position representation matrix elements

$$\Re e\, G^R(\mathbf{x}, \mathbf{x}', E) = \mathcal{P} \int_{-\infty}^{\infty} \frac{dE'}{\pi} \frac{\Im m\, G^R(\mathbf{x}, \mathbf{x}', E')}{E' - E} \tag{2.145}$$

and

$$\Im m\, G^R(\mathbf{x}, \mathbf{x}', E) = -\mathcal{P} \int_{-\infty}^{\infty} \frac{dE'}{\pi} \frac{\Re e\, G^R(\mathbf{x}, \mathbf{x}', E')}{E' - E} \ . \tag{2.146}$$

The Kramers-Kronig relations due to the retarded propagator is analytic in the upper half-plane.

The perturbation expansion of the propagator in a static potential is seen to be equivalent to the operator expansion for the Green's operator

$$\begin{aligned} \hat{G}_E &= \frac{1}{E - \hat{H}} = \frac{1}{E - \hat{H}_0 + \hat{V}} = \frac{1}{(E - \hat{H}_0)(1 - (E - \hat{H}_0)^{-1}\hat{V})} \\ &= \frac{1}{1 - (E - \hat{H}_0)^{-1}\hat{V}} \frac{1}{E - \hat{H}_0} \\ &= \left(1 + (E - \hat{H}_0)^{-1}\hat{V} + (E - \hat{H}_0)^{-1}\hat{V}(E - \hat{H}_0)^{-1}\hat{V} + \ldots\right) \frac{1}{E - \hat{H}_0} \\ &= \hat{G}_0(E) + \hat{G}_0(E)\hat{V}\hat{G}_0(E) + \hat{G}_0(E)\hat{V}\hat{G}_0(E)\hat{V}\hat{G}_0(E) + \ldots \end{aligned} \tag{2.147}$$

where

$$\hat{G}_0(E) = \frac{1}{E - \hat{H}_0} \tag{2.148}$$

is the free Green's operator.

The momentum representation of the retarded (advanced) propagator or Green's function in the energy variable can be expressed as the matrix element

$$G^{R(A)}(\mathbf{p}, \mathbf{p}', E) = <\mathbf{p}|\,\hat{G}^{R(A)}_E\,|\mathbf{p}'> \tag{2.149}$$

of the retarded (advanced) Green's operator

$$\hat{G}^{R(A)}_E = \frac{1}{E - \hat{H} \overset{+}{(-)} i0} \equiv (E - \hat{H} \overset{+}{(-)} i0)^{-1} \tag{2.150}$$

the analytical continuation from the various half-planes of the Green's operator. Other representations are obtained similarly, for example,

$$G^{R(A)}(\mathbf{x}, \mathbf{x}', E) = <\mathbf{x}|\,\hat{G}^{R(A)}_E\,|\mathbf{x}'> \ . \tag{2.151}$$

The hermitian property eq.(2.139) gives the relationship

$$[G^R(\mathbf{x}, \mathbf{x}', E)]^* = G^A(\mathbf{x}', \mathbf{x}, E^*) \tag{2.152}$$

and similarly in other representations.

Employing the resolution of the identity in terms of the eigenstates of $\hat{H}$

$$\hat{I} = \sum_\lambda |\epsilon_\lambda><\epsilon_\lambda| \tag{2.153}$$

we get the spectral representation in, for example, the position representation

$$G^{R(A)}(\mathbf{x}, \mathbf{x}', E) = \sum_\lambda \frac{\psi_\lambda(\mathbf{x})\psi^*_\lambda(\mathbf{x}')}{E - \epsilon_\lambda \overset{+}{(-)} i0} \ . \tag{2.154}$$

The Green's functions thus have singularities at the energy eigenvalues (the energy spectrum), constituting a branch cut for the continuum part of the spectrum, and simple poles for the discrete part, the latter corresponding to states which are normalizable (possible bound states of the system).

Along a branch cut the spectral function measures the discontinuity in the Green's operator

$$\begin{aligned} A(\mathbf{x}, \mathbf{x}', E) &\equiv <\mathbf{x}|i(\hat{G}_{E+i0} - \hat{G}_{E-i0})|\mathbf{x}'> \\ &= i\left(G^R(\mathbf{x}, \mathbf{x}', E) - G^A(\mathbf{x}, \mathbf{x}', E)\right) \\ &= -2\,\Im m G^R(\mathbf{x}, \mathbf{x}', E) \\ &= 2\pi \sum_\lambda \psi_\lambda(\mathbf{x})\psi^*_\lambda(\mathbf{x}')\,\delta(E - \epsilon_\lambda) \ . \end{aligned} \tag{2.155}$$

From the expression

$$A(\mathbf{x},\mathbf{x},E) = 2\pi\, Tr(\hat{P}(\mathbf{x})\delta(E-\hat{H})) = 2\pi \sum_{\lambda} |\langle\mathbf{x}|\epsilon_\lambda\rangle|^2 \delta(E-\epsilon_\lambda) \qquad (2.156)$$

we note that the diagonal elements of the spectral function, $A(\mathbf{x},\mathbf{x},E)$, is the local density of states per unit volume: the unnormalized probability per unit energy to find the particle at position $\mathbf{x}$ with energy E (or vice versa, the probability density for the particle in energy state E to be found at position $\mathbf{x}$). Employing the resolution of the identity we have

$$\int\! d\mathbf{x}\, A(\mathbf{x},\mathbf{x},E) \;=\; 2\pi \sum_{\lambda} \delta(E-\epsilon_\lambda) \;\equiv\; 2\pi\mathcal{N}(E) \qquad (2.157)$$

where $\mathcal{N}(E)$ is seen to be the number of energy levels per unit energy, and eq.(2.157) is thus the statement that the relative probability of finding the particle somewhere in space with energy E is proportional to the number of states available at that energy.

We also note the completeness relation

$$\int_\sigma \frac{dE}{2\pi}\, A(\mathbf{x},\mathbf{x}',E) \;=\; \delta(\mathbf{x}-\mathbf{x}') \qquad (2.158)$$

where the integration (and summation) is over the energy spectrum.

The position and momentum representation matrix elements of any operator are related by Fourier transformation. For the spectral operator we have (assuming the system enclosed in a box of volume V)

$$\begin{aligned} A(\mathbf{x},\mathbf{x}',E) \;&=\; \sum_{\mathbf{p}\mathbf{p}'} \langle\mathbf{x}|\mathbf{p}\rangle\, A(\mathbf{p},\mathbf{p}',E) \,\langle\mathbf{p}'|\mathbf{x}'\rangle \\ &=\; \frac{1}{V}\sum_{\mathbf{p}\mathbf{p}'} e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}-\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'} A(\mathbf{p},\mathbf{p}',E) \end{aligned} \qquad (2.159)$$

and inversely we have

$$A(\mathbf{p},\mathbf{p}',E) \;=\; \langle\mathbf{p}|\hat{A}_E|\mathbf{p}'\rangle \;=\; N^{-1}\int\! d\mathbf{x}\int\! d\mathbf{x}'\; e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}+\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'} A(\mathbf{x},\mathbf{x}',E) \qquad (2.160)$$

where the normalization depends on whether the particle is confined or not, $N = V, (2\pi\hbar)^d$.

For the diagonal momentum components of the spectral function we have

$$A(\mathbf{p},\mathbf{p},E) = 2\pi\, Tr(\hat{P}(\mathbf{p})\,\delta(E-\hat{H})) = 2\pi\sum_{\lambda} |\langle\mathbf{p}|\epsilon_\lambda\rangle|^2\delta(E-\epsilon_\lambda) \qquad (2.161)$$

describing the unnormalized probability for a particle with momentum $\mathbf{p}$ to have energy E (or vice versa). Analogously to the position representation we obtain

$$\sum_{\mathbf{p}} A(\mathbf{p},\mathbf{p},E) \;=\; 2\pi\,\mathcal{N}(E)\,. \qquad (2.162)$$

We have the momentum normalization condition

$$\int_\sigma \frac{dE}{2\pi}\, A(\mathbf{p},\mathbf{p}',E) \;=\; \left\{ \begin{array}{l} \delta(\mathbf{p}-\mathbf{p}') \\ \\ \delta_{\mathbf{p},\mathbf{p}'} \end{array} \right. \qquad (2.163)$$

depending on whether the particle is confined or not.

Let us finally discuss the analytical properties of the free propagator. Fourier transforming the free retarded propagator, eq.(2.123), we get (in three spatial dimensions for the pre-exponential factor to be correct), $\Im m E > 0$,

$$G_0^R(\mathbf{x},\mathbf{x}',E) \;=\; \frac{-m}{2\pi\hbar^2}\,\frac{e^{\frac{i}{\hbar}p_E|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} \quad , \qquad p_E = \sqrt{2mE} \qquad (2.164)$$

the solution of the spatial representation of the operator equation, eq.(2.136),

$$\left(E - \frac{\hbar^2}{2m}\Delta_{\mathbf{x}}\right) G_0(\mathbf{x},\mathbf{x}',E) \;=\; \delta(\mathbf{x}-\mathbf{x}') \qquad (2.165)$$

which is analytic in the upper half-plane.

The square root function, $\sqrt{E}$, has a half line branch cut, which according to the spectral representation, eq.(2.154), must be chosen along the positive real axis, the energy spectrum of a free particle, as we choose the lowest energy eigenvalue to have the value zero. In order for the Green's function to remain bounded for infinite separation of its spatial arguments, $|\mathbf{x}-\mathbf{x}'| \to \infty$, we must make the following choice of argument function

$$\sqrt{E} \equiv \left\{ \begin{array}{ll} \sqrt{E} & \text{for } \Re e E > 0 \\ \\ i\sqrt{|E|} & \text{for } \Re e E < 0 \end{array} \right. . \qquad (2.166)$$

rendering the free spectral function of the form

$$A_0(\mathbf{x},\mathbf{x}',E) \;=\; \frac{m}{\pi\hbar^2}\,\frac{\sin(\frac{1}{\hbar}p_E|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}\,\theta(E) \qquad (2.167)$$

and we can read off the free particle density of states, the number of energy levels per unit energy per unit volume,[13]

$$N_0(E) \;\equiv\; \frac{1}{2\pi}A_0(\mathbf{x},\mathbf{x};E) \;=\; \theta(E) \left\{ \begin{array}{ll} \sqrt{\frac{2m}{\hbar^2 E}} & d=1 \\ \\ \frac{m}{2\pi^2\hbar^2} & d=2 \\ \\ \frac{m\sqrt{2mE}}{2\pi^2\hbar^3} & d=3 \end{array} \right. \qquad (2.168)$$

[13]This result is of course directly obtained by trivial counting of the momentum states in a given energy range, because for a free particle constrained to the volume L^d, there is one momentum state per momentum volume $(2\pi\hbar/L)^d$.

for completeness we have also listed the one- and two-dimensional cases.

The spectral function for a free particle in the momentum representation follows, for example, from eq.(2.123)

$$A_0(\mathbf{p},E) \equiv A_0(\mathbf{p},\mathbf{p},E) = 2\pi\,\delta(E-\epsilon_{\mathbf{p}}) \tag{2.169}$$

and describes that a free particle with momentum $\mathbf{p}$ with certainty has energy $E=\epsilon_{\mathbf{p}}$, or vice versa.

2.8 Scattering Cross Section

We shall consider the scattering of a particle by a static potential V. At time $t=0$ we assume the particle to have momentum $\mathbf{p}'$ and are interested in the probability for finding the particle with momentum $\mathbf{p}$ at time t.

Let us first consider the Born approximation where we are only interested in the first-order correction to the propagator. According to eq.(2.98) we have

$$\begin{aligned} G_1^R(\mathbf{p},t;\mathbf{p}',t'=0) &= -\frac{<\mathbf{p}|\hat{V}|\mathbf{p}'>}{\hbar}\int_0^t d\bar{t}\; e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}(t-\bar{t})}\, e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}'}\bar{t}} \\ &= -\frac{<\mathbf{p}|\hat{V}|\mathbf{p}'>}{\hbar}\, e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}t}\, \frac{e^{\frac{i}{\hbar}t(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'})}-1}{\frac{i}{\hbar}(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'})}\,. \end{aligned} \tag{2.170}$$

To lowest order in the potential we thus have that the probability to find the particle at a later time with momentum $\mathbf{p}$, given initially that the particle had momentum $\mathbf{p}'$, is given by

$$|G_1^R(\mathbf{p},t;\mathbf{p}',0)|^2 = 2\,|<\mathbf{p}|\hat{V}|\mathbf{p}'>|^2\, \frac{1-\cos\frac{t}{\hbar}(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'})}{(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'})^2}\,. \tag{2.171}$$

We are interested in the scattering of the particle into a momentum volume containing many states, and for large times, $t\gg\hbar/\epsilon_{\mathbf{p}}$, the wildly oscillating function in eq.(2.171) is effectively a delta function, and we have

$$\begin{aligned} |G_1^R(\mathbf{p},t;\mathbf{p}',0)|^2 &= t\,\frac{2\pi}{\hbar}\,|<\mathbf{p}|\hat{V}|\mathbf{p}'>|^2\,\delta(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'}) \\ &\equiv t\,\Gamma_{\mathbf{p}\mathbf{p}'} \end{aligned} \tag{2.172}$$

and thereby for the transition probability per unit time

$$\Gamma_{\mathbf{p}\mathbf{p}'} = \frac{2\pi}{\hbar}\,|<\mathbf{p}|\hat{V}|\mathbf{p}'>|^2\,\delta(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'}) \tag{2.173}$$

i.e., Fermi's golden rule.

For the probability per unit time for the particle to be scattered into momentum states with values in the volume $\Delta\mathbf{p}$ around $\mathbf{p}$ we therefore have

$$\begin{aligned} \Gamma_{\mathbf{p}\mathbf{p}'}\frac{\Delta\mathbf{p}}{\left(\frac{2\pi\hbar}{L}\right)^3} &= L^3\int_{\Delta\mathbf{p}}\frac{d\mathbf{p}}{(2\pi\hbar)^3}\,\Gamma_{\mathbf{p}\mathbf{p}'} = \int_{\Delta\hat{\mathbf{p}}}\frac{d\hat{\mathbf{p}}}{4\pi}\int_{\Delta\epsilon_{\mathbf{p}}}d\epsilon_{\mathbf{p}}\; L^3 N_0(\epsilon_{\mathbf{p}})\Gamma_{\mathbf{p}\mathbf{p}'} \\ &= \frac{2\pi}{\hbar}\,|<\mathbf{p}|\hat{V}|\mathbf{p}'>|^2\,N_0(\epsilon_{\mathbf{p}})\,L^3\,\frac{\Delta\hat{\mathbf{p}}}{4\pi} \end{aligned} \tag{2.174}$$

where it is understood that $|\mathbf{p}'|=|\mathbf{p}|$ as demanded by energy conservation. For the probability per unit time for the particle to be scattered into a unit solid angle in the $\hat{\mathbf{p}}$-direction, $\Gamma(\hat{\mathbf{p}})$, we thus have

$$\Gamma(\hat{\mathbf{p}}) = \frac{1}{2\hbar}|<\mathbf{p}|\hat{V}|\mathbf{p}'>|^2 N_0(\epsilon_{\mathbf{p}})L^3\,. \tag{2.175}$$

The probability current density at point $\mathbf{x}$ at time t for the given initial state is

$$\begin{aligned} \mathbf{j}(\mathbf{x},t) &= \frac{\hbar}{2im}\Big(G^R(\mathbf{x},t;\mathbf{p}',0)\,\nabla_{\mathbf{x}}\,[G^R(\mathbf{x},t;\mathbf{p}',0)]^* \\ &\quad - [G^R(\mathbf{x},t;\mathbf{p}',0)]^*\,\nabla_{\mathbf{x}}\,G^R(\mathbf{x},t;\mathbf{p}',0)\Big)\,. \end{aligned} \tag{2.176}$$

In the absence of the potential, and thereby for the probability current density outside the range of the potential, we have the probability current density for a particle in state $|\mathbf{p}'>$ (recall that in eq.(2.174) box normalization is used, and the result then follows from eq.(1.320))

$$\mathbf{j}_0(\mathbf{x},t) = \frac{\mathbf{p}'}{m}\,|G_0^R(\mathbf{x},t;\mathbf{p}',0)|^2 = \frac{\mathbf{p}'}{m}\frac{1}{L^3}\,. \tag{2.177}$$

The differential cross section, $d\sigma/d\hat{\mathbf{p}}$ is defined as the probability per unit time for scattering into a unit solid angle in the $\hat{\mathbf{p}}$-direction per unit incoming flux

$$\begin{aligned} \frac{d\sigma}{d\hat{\mathbf{p}}} &\equiv \frac{\Gamma(\hat{\mathbf{p}})}{j_0} = \frac{\frac{1}{2\hbar}|<\mathbf{p}|\hat{V}|\mathbf{p}'>|^2 N_0(\epsilon_{\mathbf{p}})L^3}{\frac{p}{mL^3}} \\ &= L^6\,\frac{mN_0(\epsilon_{\mathbf{p}})}{2\hbar p}\left|\frac{1}{L^3}\int_V d\mathbf{x}\; e^{-\frac{i}{\hbar}\mathbf{x}\cdot(\mathbf{p}-\mathbf{p}')}V(\mathbf{x})\right|^2 \\ &= \left(\frac{m}{2\pi\hbar^2}\right)^2 |V(\mathbf{p}-\mathbf{p}')|^2\,. \end{aligned} \tag{2.178}$$

In a scattering experiment a beam of incoming particles is scattered by a target, and the number of particles flying off into different directions is counted. The differential cross section is therefore the quantity of interest, because it describes the relative flux of particles scattered into a given solid angle, i.e., the probability for an incoming particle per unit time to be scattered into a unit solid angle.

As an example we consider the Coulomb potential[14]

$$V_C(\mathbf{x}) = \frac{e^2}{4\pi\epsilon_0\,|\mathbf{x}|}\,, \qquad V_C(\mathbf{p}) = \frac{e^2\hbar^2}{\epsilon_0\,\mathbf{p}^2} \tag{2.179}$$

for which in lowest order, the Born approximation, we obtain the cross section

$$\frac{d\sigma_C}{d\hat{\mathbf{p}}} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left(\frac{e^2}{\epsilon_0\,p^2}\right)^2 \frac{\hbar^4}{|\hat{\mathbf{p}}-\hat{\mathbf{p}}'|^4} \,. \tag{2.180}$$

Introducing the angle between the incoming and outgoing momentum directions, $\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}' \equiv \cos\theta$, and noting that

$$|\hat{\mathbf{p}}-\hat{\mathbf{p}}'|^2 = 2\,(1-\cos\theta) = 4\sin^2\frac{\theta}{2} \tag{2.181}$$

we obtain for the differential cross section

$$\frac{d\sigma_C}{d\hat{\mathbf{p}}} = \left(\frac{e^2}{16\pi\epsilon_0}\right)^2 \frac{1}{\epsilon_{\mathbf{p}}^2\,\sin^4\frac{\theta}{2}} \,. \tag{2.182}$$

We note that the lowest order Born approximation for the Coulomb scattering cross section equals the classical Rutherford formula, which in fact is identical to the exact quantum mechanical result since the higher order terms only influence the phase of the propagator (see for example reference [6]).

For completeness we derive the expression for the differential cross section in general, i.e., beyond the Born approximation. Consider the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0$ describes a free particle $\hat{H}_0\,|\mathbf{p}\rangle = \epsilon_{\mathbf{p}}\,|\mathbf{p}\rangle$, $\epsilon_{\mathbf{p}} = \mathbf{p}^2/2m$, and $\hat{V}$ is a time-independent potential. Assuming that $\hat{H}$ has the same spectrum as $\hat{H}_0$, we can label its eigenstates similarly $\hat{H}\,|\psi_{\mathbf{p}}\rangle = \epsilon_{\mathbf{p}}\,|\psi_{\mathbf{p}}\rangle$. For an exact eigenstate we have according to eq.(2.53)

$$e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}t}|\psi_{\mathbf{p}}\rangle = e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}t}|\mathbf{p}\rangle + \frac{1}{i\hbar}\int_{-\infty}^{t}\!dt'\; e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\;\hat{V}\;e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}t'}|\psi_{\mathbf{p}}\rangle \,. \tag{2.183}$$

Expanding $\hat{V}\,|\psi_{\mathbf{p}}\rangle$ on the complete set of momentum eigenstates, we get

$$|\psi_{\mathbf{p}}\rangle = |\mathbf{p}\rangle + \frac{1}{i\hbar}\int_{-\infty}^{t}\!dt' \int\!d\mathbf{p}'\; e^{\frac{i}{\hbar}(t-t')(\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'}+i\epsilon)}\,\langle\mathbf{p}'|\hat{V}|\psi_{\mathbf{p}}\rangle\;|\mathbf{p}'\rangle \tag{2.184}$$

where we have introduced a convergence factor. Performing the integration over time gives the Lippmann-Schwinger equation,

$$|\psi_{\mathbf{p}}\rangle = |\mathbf{p}\rangle + \int\!d\mathbf{p}'\;\frac{\langle\mathbf{p}'|\hat{V}|\psi_{\mathbf{p}}\rangle}{\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}'}+i\epsilon}\,|\mathbf{p}'\rangle \,. \tag{2.185}$$

[14] We adopt the standard SI units.

In the position representation we obtain

$$\psi_{\mathbf{p}}(\mathbf{x}) = \frac{e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}}{(2\pi\hbar)^{d/2}} + \int\!d\mathbf{x}'\;G_0^R(\mathbf{x},\mathbf{x}',\epsilon_{\mathbf{p}})\,V(\mathbf{x}')\,\psi_{\mathbf{p}}(\mathbf{x}') \tag{2.186}$$

where the free retarded propagator was obtained in eq.(2.164). We are free to drop the normalization factor since $|\psi_{\mathbf{p}}\rangle$ and $|\mathbf{p}\rangle$ have the same normalization, because the time evolution, eq.(2.53), of course is unitary. Integrating eq.(2.183) with an envelope function we obtain

$$|\psi_g(t)\rangle = |\phi_g(t)\rangle + \frac{1}{i\hbar}\int_{-\infty}^{t}\!dt'\; e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}\;\hat{V}\;e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}t'}|\psi_g(t')\rangle \tag{2.187}$$

where

$$|\psi_g(t)\rangle \equiv \int_0^\infty\!d\epsilon_{\mathbf{p}}\,g(\epsilon_{\mathbf{p}})\,e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}t}|\psi_{\mathbf{p}}\rangle\,, \qquad |\phi_g(t)\rangle \equiv \int_0^\infty\!d\epsilon_{\mathbf{p}}\,g(\epsilon_{\mathbf{p}})\,e^{-\frac{i}{\hbar}\epsilon_{\mathbf{p}}t}|\mathbf{p}\rangle \tag{2.188}$$

and the envelope function g is assumed a smooth function peaked at some energy value. Far in the past the wave packet in eq.(2.187) therefore has free evolution toward the target potential as described by the first term on the right side of eq.(2.187), and at later times a scattered wave develops, the second term on the right side. Instead of performing the wave packet analysis of scattering, we note that we can calculate the scattering properties from the asymptotic form of the exact solution to the stationary Schrödinger equation, $|\mathbf{x}| \to \infty$, as easily obtained from eq.(2.186):

$$\psi_{\mathbf{p}}(\mathbf{x}) = e^{\frac{i}{\hbar}pz} + f(\theta)\,\frac{e^{\frac{i}{\hbar}|\mathbf{p}|\,|\mathbf{x}|}}{|\mathbf{x}|} \tag{2.189}$$

where

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int\!d\mathbf{x}'e^{-\frac{i}{\hbar}\frac{|\mathbf{p}|}{|\mathbf{x}|}\mathbf{x}\cdot\mathbf{x}'}\;V(\mathbf{x})\,\psi_{\mathbf{p}}(\mathbf{x}') \tag{2.190}$$

and we have chosen the $\hat{z}$-direction along the direction of the momentum of the incoming particle, and the scattering angle, θ, is the angle between the incoming momentum and the direction to the point $\mathbf{x}$. Calculating the probability current density in the scattered wave relative to the incident wave, we get for the differential cross section

$$\frac{d\sigma}{d\hat{\mathbf{p}}} = |f(\theta)|^2 \,. \tag{2.191}$$

2.9 Inversion and Time-Reversal Symmetry

If we change the sense of positive direction of the coordinate axes of a reference frame, we get an equivalent description of space in which points in space change label according to $\mathbf{x} \to -\mathbf{x}$.[15] The unitary operator relating the two descriptions obtained by spatial inversion through a point, here chosen as the origin, is specified by

$$\hat{U}_P\,|\mathbf{x}> \;=\; e^{i\varphi(\mathbf{x})}|-\mathbf{x}> \tag{2.192}$$

The inversion or reflection operator is equivalently, up to a phase transformation, specified by the transformation property of the position operator

$$\hat{U}_P^{-1}\,\hat{\mathbf{x}}\,\hat{U}_P \;=\; -\hat{\mathbf{x}} \tag{2.193}$$

or

$$\hat{\mathbf{x}}\,\hat{U}_P\,|\mathbf{x}> \;=\; -\mathbf{x}\,\hat{U}_P\,|\mathbf{x}> \;. \tag{2.194}$$

We could also define the inversion operator on an arbitrary state, with the phase choice $\hat{U}_P^2 \;=\; \hat{I}$, by

$$<\mathbf{x}|\hat{U}_P^\dagger\,|\psi> \;=\; <-\mathbf{x}|\psi> \quad \text{or equivalently} \quad \hat{U}_P\,\psi(\mathbf{x}) \;=\; \psi(-\mathbf{x})\;. \tag{2.195}$$

By construction of the complementary operator (using the inversion changed basis $<x_i| \to <\underline{x}_i| = <x_i|\hat{U}_P^\dagger$, we encounter, compared to section 1.4, the change $\hat{\mathcal{V}} \to \hat{\underline{\mathcal{V}}} = \exp\{-id\hat{p}\}$), we have for the momentum operator

$$\hat{\mathbf{p}}\,\hat{U}_P\,|\mathbf{p}> \;=\; -\mathbf{p}\,\hat{U}_P\,|\mathbf{p}> \quad \text{or equivalently} \quad \hat{U}_P^{-1}\,\hat{\mathbf{p}}\,\hat{U}_P \;=\; -\hat{\mathbf{p}}\;. \tag{2.196}$$

This is also immediately verified by exploiting the property the transformation function $<\mathbf{p}|-\mathbf{x}> = <-\mathbf{p}|\mathbf{x}>$

$$\begin{aligned} <\mathbf{p}|\hat{U}_P^\dagger|\psi> &= \int\! d\mathbf{x}\, <\mathbf{p}|\mathbf{x}><\mathbf{x}|\hat{U}_P^\dagger|\psi> = \int\! d\mathbf{x}\, <\mathbf{p}|\mathbf{x}><-\mathbf{x}|\psi> \\ &= \int\! d\mathbf{x}\, <\mathbf{p}|-\mathbf{x}><\mathbf{x}|\psi> = \int\! d\mathbf{x}\, <-\mathbf{p}|\mathbf{x}><\mathbf{x}|\psi> \\ &= <-\mathbf{p}|\psi> \end{aligned} \tag{2.197}$$

i.e.,

$$\hat{U}_P\,\psi(\mathbf{p}) \;=\; \psi(-\mathbf{p})\;. \tag{2.198}$$

Position and momentum vectors change sign under reflection, and are called polar vectors, whereas angular momentum $\hat{\mathbf{L}} = \hat{\mathbf{x}}\times\hat{\mathbf{p}}$ is invariant, $\hat{U}_P^{-1}\,\hat{\mathbf{L}}\,\hat{U}_P = \hat{\mathbf{L}}$, and are called an axial vector or pseudo-vector. The spin up and down states of an electron are defined relative to a quantization axis, say the direction of the magnetic field in the Stern-Gerlach apparatus. Since the magnetic field is described by an axial vector it is invariant under space inversion, and consequently we have that the spin is invariant under space inversion

$$\hat{U}_P^{-1}\,\hat{\mathbf{s}}\,\hat{U}_P \;=\; \hat{\mathbf{s}}. \tag{2.199}$$

[15] The spatial inversion or reflection through a point interchanges right- and left-handed coordinate systems.

Since $\hat{U}_P^2$ commutes with both the position and momentum operators, $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}$, it is proportional to the identity operator, and since $\hat{U}_P$ is unitary the proportionality factor is just a phase factor. With the phase choice $\hat{U}_P^2 = \hat{I}$,[16] we have that the reflection or inversion operator is also hermitian, $\hat{U}_P^\dagger \;=\; \hat{U}_P \;=\; \hat{U}_P^{-1}$. For $\hat{U}_P^2 \;=\; \hat{I}$, the eigenvalues of the reflection operator is ± 1, and are called the parity.

Using eq.(1.317) we note that

$$\int\!\frac{d\mathbf{x}'d\mathbf{p}'}{(4\pi\hbar)^d}\; e^{\frac{i}{\hbar}\mathbf{x}'\cdot\hat{\mathbf{p}}-\frac{i}{\hbar}\mathbf{p}'\cdot\hat{\mathbf{x}}}\;|\mathbf{x}> \;=\; |-\mathbf{x}> \tag{2.200}$$

and similarly for momentum states

$$\int\!\frac{d\mathbf{x}'d\mathbf{p}'}{(4\pi\hbar)^d}\; e^{\frac{i}{\hbar}\mathbf{x}'\cdot\hat{\mathbf{p}}-\frac{i}{\hbar}\mathbf{p}'\cdot\hat{\mathbf{x}}}\;|\mathbf{p}> \;=\; |-\mathbf{p}> \tag{2.201}$$

and for the above phase choice we have

$$\hat{U}_P \;=\; \int\!\frac{d\mathbf{x}'d\mathbf{p}'}{(4\pi\hbar)^d}\; e^{\frac{i}{\hbar}\mathbf{x}'\cdot\hat{\mathbf{p}}-\frac{i}{\hbar}\mathbf{p}'\cdot\hat{\mathbf{x}}}\;. \tag{2.202}$$

For a Hamiltonian invariant under reflection[17]

$$\hat{U}_P\,\hat{H}\,\hat{U}_P^{-1} \;=\; \hat{H} \tag{2.203}$$

we have the properties of the transformation functions

$$<\mathbf{x},t|\mathbf{x}',t'> \;=\; <-\mathbf{x},t|-\mathbf{x}',t'> \quad , \quad <\mathbf{p},t|\mathbf{p}',t'> \;=\; <-\mathbf{p},t|-\mathbf{p}',t'>\;. \tag{2.204}$$

Finally we wish to derive the consequences of time-reversal invariance for the transformation functions. If the potential in the Hamiltonian eq.(1.33) is time independent, we can immediately infer that if $\psi(\mathbf{x},t)$ is a solution of the Schrödinger equation, eq.(1.32), so is $\overline{\psi}(\mathbf{x},t) \equiv \psi^*(\mathbf{x},-t)$. Comparing the time evolution on integral form (eq.(1.5) or eq.(1.351)) of $\psi(\mathbf{x},t)$ and $\overline{\psi}(\mathbf{x},t)$, we discover that for the considered Hamiltonian the transformation function has the following property

$$<\mathbf{x},t|\mathbf{x}',t'>^* \;=\; <\mathbf{x},-t|\mathbf{x}',-t'> \tag{2.205}$$

which is equivalent to

$$<\mathbf{x},t|\mathbf{x}',t'> \;=\; <\mathbf{x}',t|\mathbf{x},t'>\;. \tag{2.206}$$

For the transformation function in the momentum representation we then get

$$<\mathbf{p},t|\mathbf{p}',t'> \;=\; <-\mathbf{p}',t|-\mathbf{p},t'>\;. \tag{2.207}$$

[16] The group of reflections in a point has only two elements, $\hat{U}_P$ and $\hat{I}$.

[17] In this case $\hat{U}_P$ is a constant of the motion.

Time reversal interchanges the initial and final states, and reverses the direction of motion.

The Schrödinger equation is clearly not invariant with respect to time inversion $t \to -t$. However, by in addition subduing the wave function to complex conjugation we generate the motion-reversed solution[18]

$$\hat{T}\,\psi(\mathbf{x},t) \;=\; \psi^*(\mathbf{x},-t)\,. \tag{2.208}$$

In the position representation we can contemplate a motion picture of the time evolution of a system, say for simplicity of the probability density distribution for a particle $P(\mathbf{x},t)$. The time-reversal invariance of a systems dynamics can then vividly be expressed in the active point of view[19] as the statement: the time evolution of the probability density obtained by watching the picture played backwards, the motion-reversed state, is a possible solution of the Schrödinger equation for the system. It is readily shown that for the considered Hamiltonian this solution is given by $\overline{P}(\mathbf{x},t) \equiv |\overline{\psi}(\mathbf{x},t)|^2 = |\psi^*(\mathbf{x},-t)|^2$ and represents the time-reversed motion of the probability density. We speak of $\psi^*(\mathbf{x},-t)$ as the time-reversed solution of the original solution, $\psi(\mathbf{x},t)$, of the Schrödinger equation.

In quantum mechanics we thus encounter a symmetry which falls outside the scheme of being represented by a unitary operator, and more importantly by a linear operator. This is the possible symmetry connected with the dynamics of the system, and we now give a general discussion of time-reversal invariance. A system is said to respect time-reversal symmetry if there exists an operator $\hat{T}$ for which ($|T\psi> \equiv \hat{T}|\psi>$)

$$<\psi_f|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|\psi_i> \;=\; <T\psi_i|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|T\psi_f>\,. \tag{2.209}$$

Equivalently it is said that the dynamics of a system is time-reversal invariant if the transition amplitude from state $|\psi_i>$ at time t_i to state $|\psi_f>$ at time t_f equals the transition amplitude from state $|T\psi_f>$ at time t_i to state $|T\psi_i>$ at time t_f.[20]

In view of the relation eq.(C.6), established in appendix C, applied to the linear operator $\exp\{-i\hat{H}(t_f-t_i)/\hbar\}$, the dynamics of a system is thus time-reversal invariant if there exists an antiunitary operator $\hat{T}$ which commutes with the Hamiltonian

$$\hat{T}\,\hat{H}\,\hat{T}^{-1} \;=\; \hat{H}\,. \tag{2.210}$$

[18]This is explicitly shown in exercise 4.5 on page 175.

[19]In reality, reversing the direction of time is not a viable alternative. The passive point of view corresponds to using backward-running clocks (reversed direction for measuring the progression of time), in which case the Schrödinger equation reads

$$-i\hbar\,\frac{d|\overline{\psi}(t)>}{dt} \;=\; \hat{H}\,|\overline{\psi}(t)>\,.$$

[20]By proper phase choice of the states in eq.(2.209) the appearance of absolute value signs are superfluous.

Let us construct the time-reversal operator for the case of a particle in a time-independent potential V for which we have the Hamiltonian

$$\hat{H} \;=\; \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}})\,. \tag{2.211}$$

We immediately find that in the position representation the antiunitary operation of complex conjugation[21]

$$\hat{K}_{(x)}\,\psi(\mathbf{x}) \;\equiv\; \psi^*(\mathbf{x}) \tag{2.212}$$

commutes with the Hamiltonian. In view of the wave function being the expansion coefficients on the position basis (recall eq.(1.132))

$$|\psi> \;=\; \int\! d\mathbf{x}\;\psi(\mathbf{x})\,|\mathbf{x}> \tag{2.213}$$

we have for the complex conjugate operator with respect to the position basis (see appendix C)

$$\hat{K}_{(x)}\,|\psi> \;\equiv\; \int\! d\mathbf{x}\;\psi^*(\mathbf{x})\,|\mathbf{x}> \tag{2.214}$$

and because

$$<\mathbf{x}|K_{(x)}\psi> \;\equiv\; <\mathbf{x}|\hat{K}_{(x)}|\psi> \;=\; \psi^*(\mathbf{x})\,. \tag{2.215}$$

we have that for a spinless particle the time-reversal operator is simply the complex conjugation operator defined with respect to the position basis, $\hat{T} = \hat{K}_{(x)}$. We note that for a spinless particle we have $\hat{T}^2 = \hat{I}$.

Since the time-reversal operator in the position representation is the complex conjugation operator, we immediately obtain the transformation properties of the position and momentum operators ($\hat{T}_{(x)}(-i\hbar\nabla_{\mathbf{x}})\hat{T}_{(x)}^{-1} = i\hbar\nabla_{\mathbf{x}}$) under time-reversal invariance

$$\hat{T}\,\hat{\mathbf{x}}\,\hat{T}^{-1} \;=\; \hat{\mathbf{x}} \quad,\quad \hat{T}\,\hat{\mathbf{p}}\,\hat{T}^{-1} \;=\; -\hat{\mathbf{p}}\,. \tag{2.216}$$

Transforming to the momentum representation (with the convention eq.(1.320) for the phase factor) we find that the time-reversed state in the momentum representation is given by[22]

$$\hat{T}\,\psi(\mathbf{p}) \;=\; \psi^*(-\mathbf{p})\,. \tag{2.217}$$

The time-reversed state is thus the motion-reversed state.

For the current density we have (see eq.(1.357) on page 68)

$$<\hat{\mathbf{j}}>_{\overline{\psi}} \;=\; -<\hat{\mathbf{j}}>_{\psi}\,. \tag{2.218}$$

For a time-reversal invariant Hamiltonian we obtain for the current density operator in the Heisenberg picture the relation (we are inverting time with respect to $t=0$)

$$\hat{T}\,\hat{\mathbf{j}}(\mathbf{x},t)\,\hat{T}^\dagger \;=\; -\,\hat{\mathbf{j}}(\mathbf{x},-t)\,. \tag{2.219}$$

[21]We are discussing the properties of the wave function at the moment in time of inversion. If we wish to discuss the action of the time-reversal operator at a different time we must also reverse the direction of time, see eq.(2.208).

[22]The time-reversal operator in the momentum representation is thus not simply the complex conjugation operator with respect to the momentum basis, but involves the substitution $\mathbf{p} \to -\mathbf{p}$.

Exercise 2.7 *Verify the transformation properties eq.(2.216) using the momentum representation.*

In particular we note that with the phase choice we have made (see appendix C) we have

$$\hat{T}\,|\mathbf{x}> \;=\; |\mathbf{x}> \tag{2.220}$$

and eq.(2.206) is a special case of eq.(2.209). Similarly, since

$$\hat{T}|\mathbf{p}> \;=\; \hat{T}\int\! d\mathbf{x}\; <\mathbf{x}|\mathbf{p}>\,|\mathbf{x}> \;=\; \int\! d\mathbf{x}\; <\mathbf{x}|\mathbf{p}>^*\,|\mathbf{x}> \;=\; |-\mathbf{p}> \tag{2.221}$$

we recover that eq.(2.207) is a special case of eq.(2.209).

Exercise 2.8 *Discuss time-reversal symmetry for a system exposed to an external magnetic field.*

The orbital angular momentum transforms under time reversal according to eq.(2.216) as

$$\hat{T}\,\hat{\mathbf{L}}\,\hat{T}^\dagger \;=\; -\hat{\mathbf{L}}\,. \tag{2.222}$$

Since the magnetic field changes sign under time reversal (the sources generating the field are supposed to have their motion reversed) we have for the transformation properties of the spin under time reversal

$$\hat{T}\,\hat{\mathbf{s}}\,\hat{T}^\dagger \;=\; -\hat{\mathbf{s}}.\,. \tag{2.223}$$

Using the standard basis in the operator spin space (recall exercise 1.9 on page 49) whose matrix representation are the Pauli matrices, we have

$$\hat{K}_{(x)}\,\hat{s}_x\,\hat{K}_{(x)} \;=\; \hat{s}_x \;,\quad \hat{K}_{(x)}\,\hat{s}_y\,\hat{K}_{(x)} \;=\; -\hat{s}_y \;,\quad \hat{K}_{(x)}\,\hat{s}_z\,\hat{K}_{(x)} \;=\; \hat{s}_z \tag{2.224}$$

and for the spin part $\hat{T}_\sigma$ of the time-reversal operator, $\hat{T} = \hat{T}_\sigma\,\hat{K}_{(x)}$, we have

$$\hat{T}_\sigma\,\hat{\mathbf{x}}\,\hat{T}_\sigma^\dagger \;=\; \hat{\mathbf{x}} \;,\quad \hat{T}_\sigma\,\hat{\mathbf{p}}\,\hat{T}_\sigma^\dagger \;=\; \hat{\mathbf{p}} \tag{2.225}$$

and

$$\hat{T}_\sigma\,\hat{s}_x\,\hat{T}_\sigma^\dagger \;=\; -\hat{s}_x \;,\quad \hat{T}_\sigma\,\hat{s}_y\,\hat{T}_\sigma^\dagger \;=\; \hat{s}_y \;,\quad \hat{T}_\sigma\,\hat{s}_z\,\hat{T}_\sigma^\dagger \;=\; -\hat{s}_z\,. \tag{2.226}$$

The last set of equalities describes a rotation in spin space through the angle π around the y-axis, and according to exercise 1.11 we have (up to a phase factor)

$$\hat{T}_\sigma \;=\; e^{\frac{i}{\hbar}\pi\hat{s}_y}\,. \tag{2.227}$$

For the spin-1/2 case we have the matrix representation

$$\underline{\underline{T}} \;=\; i\sigma_y\,. \tag{2.228}$$

The time-reversal operator for a spin-1/2 particle is seen to satisfy $\hat{T}^2 \;=\; -\hat{I}$ (independent of phase convention and choice of representation).

We note that a spin-orbit coupling, $\hat{\mathbf{s}}\cdot\hat{\mathbf{L}}$, does not break the time-reversal invariance of a Hamiltonian.

2.10 The Density Matrix

When a particle interacts with an environment which has its own dynamics, i.e., its effect upon the particle can not be described by potentials, we need to develop the diagrammatic technique for the density matrix since statistical averages with respect to the environment are taken over the distribution function. In this section we develop the density-matrix formalism for a particle interacting with a potential, which we shall need for the treatment of a particle moving in a random potential. The treatment of a quantum environment is given in chapter 6.

We assume, that at time t' the particle is in the state ρ' described by the statistical operator $\hat{\rho}' \equiv \hat{\rho}(t')$. For the statistical operator at time t we have according to eq.(1.368)

$$\hat{\rho}(t) \;=\; \hat{U}(t,t')\,\hat{\rho}'\,\hat{U}^\dagger(t,t')\,. \tag{2.229}$$

The density matrix in the position representation is

$$\rho(\mathbf{x},\mathbf{x}',t) \;\equiv\; <\mathbf{x}|\hat{\rho}(t)|\mathbf{x}'> \;=\; Tr(\hat{\rho}(t)|\mathbf{x}'><\mathbf{x}|)\,. \tag{2.230}$$

The diagonal element $\rho(\mathbf{x},\mathbf{x},t)$ is the probability density to find the particle at position $\mathbf{x}$ at time t

$$\rho(\mathbf{x},\mathbf{x},t) = Tr(\hat{\rho}(t)\hat{P}(\mathbf{x})) = Tr(\hat{\rho}(t_r)\hat{P}(\mathbf{x},t)) \equiv P(\mathbf{x},t)\,. \tag{2.231}$$

Here $\hat{\rho}(t_r)$ is the statistical operator at the reference time t_r, where the Heisenberg and Schrödinger pictures are chosen to coincide. We can also express the diagonal elements of the density matrix in terms of the density operator

$$P(\mathbf{x},t) = \rho(\mathbf{x},\mathbf{x},t) = Tr(\hat{\rho}(t)\hat{n}(\mathbf{x})) = Tr(\hat{\rho}(t_r)\hat{n}(\mathbf{x},t)) \equiv n(\mathbf{x},t)\,. \tag{2.232}$$

The diagonal elements of the density matrix exemplify the simplest kind of a consistent family of histories, referring only to one moment in time. The propositions in the family are of the form (suppressing the reference to the initial state) *the particle is at position* $\mathbf{x}$ *at time* t, and have their associated probability density

$$p_\rho((\mathbf{x}t)) \;=\; \rho(\mathbf{x},\mathbf{x},t) \;=\; P(\mathbf{x},\mathbf{t})\,. \tag{2.233}$$

We can also consider the two-time history, that the particle is at position $\mathbf{x}'$ at time t', and at position $\mathbf{x}$ at the later time t, given the state of the particle is known to be ρ at some moment in time in the past. The associated probability of this history is (choosing the moment in time where the state is ρ as our reference time $\hat{\rho} \equiv \hat{\rho}(t_r)$)

$$\begin{aligned} p_\rho((\mathbf{x}t),(\mathbf{x}'t')) &= Tr(\hat{n}(\mathbf{x}',t')\,\hat{\rho}\,\hat{n}(\mathbf{x}',t')\,\hat{n}(\mathbf{x},t)) \\ &= <\mathbf{x}',t'|\hat{n}(\mathbf{x},t)|\mathbf{x}',t'>\,\rho(\mathbf{x}',\mathbf{x}',t') \\ &= |G^R(\mathbf{x},t;\mathbf{x}',t')|^2\,\rho(\mathbf{x}',\mathbf{x}',t') \\ &= P(\mathbf{x},t;\mathbf{x}',t')\,\rho(\mathbf{x}',\mathbf{x}',t') \\ &= P(\mathbf{x},t;\mathbf{x}',t')\,p_\rho(\mathbf{x}',t') \end{aligned} \qquad (2.234)$$

which of course is expressible as the probability that the particle in state ρ will be at position $\mathbf{x}'$ at time t' multiplied by the conditional probability for the particle to be at position $\mathbf{x}$ at time t given it was at position $\mathbf{x}'$ at time t'.

Exercise 2.9 *Show that for the conditional probability density we have the formula*

$$P(\mathbf{x},t;\mathbf{x}',t') = Tr(\delta(\mathbf{x}-\hat{\mathbf{x}}(t))\,\delta(\mathbf{x}'-\hat{\mathbf{x}}(t'))) \qquad (2.235)$$

where $\hat{\mathbf{x}}(t)$ is the position operator in the Heisenberg picture.

Inserting complete sets of position eigenstates in eq.(2.229), we get the integral equation determining the time evolution of the density matrix

$$\rho(\mathbf{x},\mathbf{x}',t) = \int\! d\tilde{\mathbf{x}} \int\! d\tilde{\mathbf{x}}'\; J(\mathbf{x},\mathbf{x}',t;\tilde{\mathbf{x}},\tilde{\mathbf{x}}',t')\,\rho(\tilde{\mathbf{x}},\tilde{\mathbf{x}}',t') \qquad (2.236)$$

which is specified in terms of the propagator of the density matrix

$$\begin{aligned} J(\mathbf{x},\mathbf{x}',t;\tilde{\mathbf{x}},\tilde{\mathbf{x}}',t') &= <\tilde{\mathbf{x}}'|\hat{U}^\dagger(t,t')|\mathbf{x}'><\mathbf{x}|\hat{U}(t,t')|\tilde{\mathbf{x}}> \\ &= <\tilde{\mathbf{x}}',t'|\mathbf{x}',t><\mathbf{x},t|\tilde{\mathbf{x}},t'> \\ &= G^*(\mathbf{x}',t;\tilde{\mathbf{x}}',t')\,G(\mathbf{x},t;\tilde{\mathbf{x}},t') \\ &= G(\tilde{\mathbf{x}}',t';\mathbf{x}',t)\,G(\mathbf{x},t;\tilde{\mathbf{x}},t') \end{aligned} \qquad (2.237)$$

and the density matrix at time t'

$$\rho(\mathbf{x},\mathbf{x}',t') = <\mathbf{x}|\hat{\rho}(t')|\mathbf{x}'> \equiv \rho'(\mathbf{x},\mathbf{x}') \,. \qquad (2.238)$$

Expressing the density matrix propagator, J, in terms of the retarded and advanced propagators we have

$$J(\mathbf{x},\mathbf{x}',t;\tilde{\mathbf{x}},\tilde{\mathbf{x}}',t') = \begin{cases} G^R(\mathbf{x},t;\tilde{\mathbf{x}},t')\,G^A(\tilde{\mathbf{x}}',t';\mathbf{x}',t) & \text{for } t>t' \\ G^A(\mathbf{x},t;\tilde{\mathbf{x}},t')\,G^R(\tilde{\mathbf{x}}',t';\mathbf{x}',t) & \text{for } t<t' \,. \end{cases} \qquad (2.239)$$

Since

$$\begin{aligned} J(\mathbf{x},\mathbf{x},t;\mathbf{x}',\mathbf{x}',t') &= G^R(\mathbf{x},t;\mathbf{x}',t')\,G^A(\mathbf{x}',t';\mathbf{x},t) = |G^R(\mathbf{x},t;\mathbf{x}',t')|^2 \\ &\equiv P(\mathbf{x},t\,;\mathbf{x}',t') \end{aligned} \qquad (2.240)$$

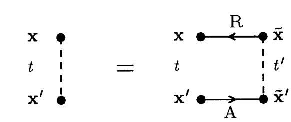
the spatial diagonal elements of the density matrix propagator, $J(\mathbf{x},\mathbf{x},t;\mathbf{x}',\mathbf{x}',t')$, have the simple physical interpretation: It is the conditional probability density for the particle to be found at position $\mathbf{x}$ at time t, given that it was at position $\mathbf{x}'$ at time t'.[23]

The probability distribution at time t, $P(\mathbf{x},t) = \rho(\mathbf{x},\mathbf{x},t)$, can not, according to eq.(2.236), be expressed as a functional of the probability distribution at an earlier time, as off-diagonal elements of the density matrix are of importance. In particular we note the failure of the Markovian property in general for primitive histories

$$p_\rho((\mathbf{x},t)) = \rho(\mathbf{x},\mathbf{x},t) \neq \int\! d\mathbf{x}'\; p_\rho((\mathbf{x}t),(\mathbf{x}'t')) = \int\! d\mathbf{x}'\; P(\mathbf{x},t;\mathbf{x}',t')\,p_\rho((\mathbf{x}',t')) \qquad (2.241)$$

except for the case where the state ρ' corresponds to a state of definite position.

For the simplest of environments, that of an external potential, we have diagrammatically for the density matrix (we assume $t > t'$)

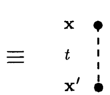


(2.242)

and the dictionary for transcribing the diagrams is according to eq.(2.236) as follows:

A stipulated vertical line represents the density matrix:

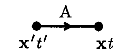
$\rho(\mathbf{x},\mathbf{x}',t) \equiv$



(2.243)

[23] This is also immediately obtained from eq.(2.236) by noting that the state for a particle at position $\mathbf{x}'$ is described by the statistical operator $\hat{\rho} = |\mathbf{x}'><\mathbf{x}'|$, and therefore by the density matrix $\rho(\tilde{\mathbf{x}},\tilde{\mathbf{x}}') = <\tilde{\mathbf{x}}|(|\mathbf{x}'><\mathbf{x}'|)|\tilde{\mathbf{x}}'> = \delta(\tilde{\mathbf{x}}-\mathbf{x}')\,\delta(\tilde{\mathbf{x}}'-\mathbf{x}')$.

and we have introduced thick solid lines to represent the particle propagators in the presence of the potential, for example the advanced propagator is depicted as



$$= \; G^A(\mathbf{x},t;\mathbf{x}',t') \quad . \tag{2.244}$$

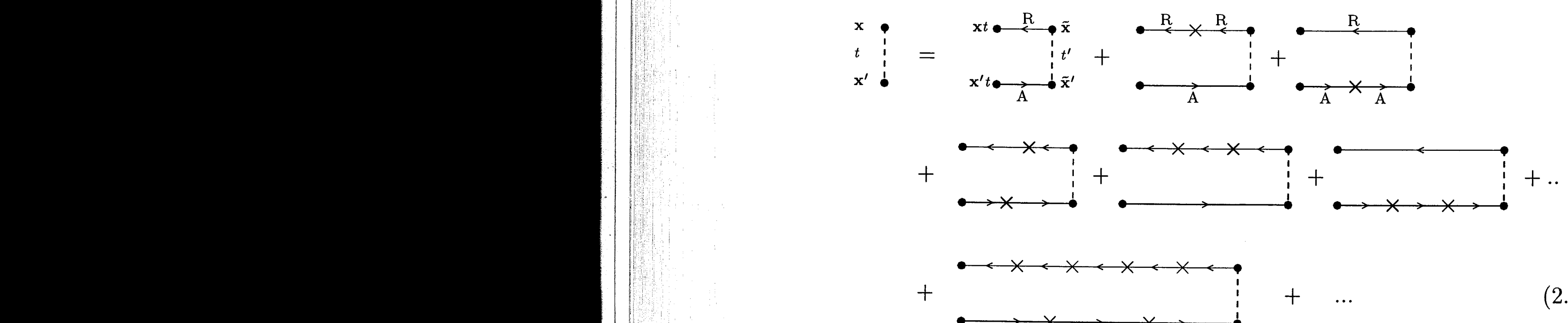
In accordance with eq.(2.236), spatial integrations over the initial density-matrix coordinates are implied.

The perturbative expansion and diagrammatic representation of the density-matrix propagator, and thereby also of the density matrix, is immediately obtained because we know the perturbative expansion for the retarded propagator (and thereby also the one for the advanced propagator)

$$\begin{aligned} J(\mathbf{x},\mathbf{x}',t;\tilde{\mathbf{x}},\tilde{\mathbf{x}}',t') \;=\; & \sum_{n,m=0}^{\infty}\left(\frac{1}{\hbar}\right)^{n+m}\int\prod_{n'=1}^{n}dx_{n'}\int_{-\infty}^{\infty}\prod_{n'=1}^{n}dt_{n'}\int\prod_{m'=1}^{m}d\tilde{x}_{m'}\int_{-\infty}^{\infty}\prod_{m'=1}^{m}d\tilde{t}_{m'} \\ & G_0^R(\mathbf{x},t;\mathbf{x}_n,t_n)G_0^R(\mathbf{x}_n,t_n;\mathbf{x}_{n-1},t_{n-1})..G_0^R(\mathbf{x}_1,t_1;\tilde{\mathbf{x}},t') \\ & G_0^A(\tilde{\mathbf{x}}',t';\tilde{\mathbf{x}}_m,\tilde{t}_m)G_0^A(\tilde{\mathbf{x}}_m,\tilde{t}_m;\tilde{\mathbf{x}}_{m-1},\tilde{t}_{m-1})..G_0^A(\tilde{\mathbf{x}}_1,\tilde{t}_1;\mathbf{x}',t) \\ & V(\tilde{\mathbf{x}}_m,\tilde{t}_{m-1})V(\mathbf{x}_{m-1},\tilde{t}_{m-1})..V(\tilde{\mathbf{x}}_1,\tilde{t}_1) \\ & V(\mathbf{x}_n,t_n)V(\mathbf{x}_{n-1},t_{n-1})..V(\mathbf{x}_1,t_1) \end{aligned} \tag{2.245}$$

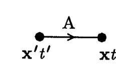
where we have assumed that the time t is later than t' (for the opposite sequence the advanced and retarded labels should be interchanged).

Diagrammatically we have for the density matrix for a particle in a potential the perturbative expansion



(2.246)

where we as usual use thin solid lines to represent the free particle propagators; for example, the advanced free propagator is depicted as



$$= \; G_0^A(\mathbf{x},t;\mathbf{x}',t') \, . \tag{2.247}$$

In accordance with the derivation, integration over interaction space-time points should be performed, and spatial integrations over the initial density matrix coordinates. With the chosen conventions there are no additional factors, so with each diagram is associated the same trivial factor of +1.

The double line diagrams for the density matrix, with the retarded propagator exclusively appearing on the upper line, and the advanced propagator exclusively on the lower line, are generic to quantum dynamics, reflecting the presence of both $\hat{U}$ and $\hat{U}^\dagger$ in the time evolution of the density matrix. The diagonal elements of the density matrix, which are real numbers, are expressed as sums of complex numbers, but they come in pairs that are each other's complex conjugates as is characteristic of quantum mechanical interference.

If the density matrix at some point in time factorizes; i.e., the system is prepared in some pure state ψ, $\rho(\mathbf{x},\mathbf{x}',t') = \psi(\mathbf{x})\,\psi^*(\mathbf{x}')$, the motion of the particle in a potential is uniquely determined by the propagator.

For a statistical operator diagonal in the energy representation

$$\hat{\rho} \;=\; \sum_{\lambda} \rho(\epsilon_\lambda)\,|\epsilon_\lambda\rangle\langle\epsilon_\lambda| \tag{2.248}$$

we obtain from eq.(2.156) the relation between the density matrix and the combination of the energy distribution function and the spectral weight

$$\int_{-\infty}^{\infty}\frac{dE}{2\pi}\,\rho(E)A(\mathbf{x},\mathbf{x}';E) \;=\; \langle\mathbf{x}|\hat{\rho}|\mathbf{x}'\rangle \;=\; \rho(\mathbf{x},\mathbf{x}') \, . \tag{2.249}$$

For the diagonal elements, $\mathbf{x}' = \mathbf{x}$, the equation has the interpretation: the probability of finding the particle at position $\mathbf{x}$ is the probability to find the particle at position $\mathbf{x}$ *given* it has energy E, A($\mathbf{x}$,$\mathbf{x}$;E), times the probability it has energy E, $\rho(E)$, summed over all possible energy values.

Exercise 2.10 *Show, by taking the momentum matrix element of the von Neumann equation, eq.(1.369), that the density matrix for a free particle in the momentum representation satisfies the equation*

$$\frac{\partial\rho(\mathbf{p},\mathbf{p}',t)}{\partial t} - \frac{i}{\hbar}\left(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'}\right)\rho(\mathbf{p},\mathbf{p}',t) \;=\; 0 \, . \tag{2.250}$$