10   Observables and Propagators

In the past lectures we have considered the properties of a number of field the-
ories that describe physical systems isolated from the outside world. However,
the only way to investigate the properties of a physical system is to interact with
it. Thus, we must consider physical systems which somehow are coupled to their
surroundings. We will have two situations in mind. In one case, we will look at
the problem of the interaction of states of an isolated system, *i.e.,* a scattering
problem. In this case we prepare states (or wave packets) which are sufficiently
far apart so that their mutual interactions can be neglected. The prototype
is the scattering of particles off a target or each other in a particle accelerator
experiment. Here the physical properties are encapsulated in a suitable set of
cross sections. In the second case we will imagine that we want to understand
that properties of a large system "from outside", and we will consider the role of
small external perturbations. Here we will develop a general approach, known
as Linear Response Theory. We will couch our results in terms of a suitable set
of susceptibilities. This is the typical situation of interest in an experiment in a
condensed matter system.

In both cases, all quantities of physical interest will be derived from a suitably
defined Green function or propagator. Our task will be twofold. First we will
determine the general expected properties of the propagators, in particular their
analytic properties. Second we will see that their analytic properties largely
determine the behavior of cross sections and susceptibilities.

10.1   The Propagator in Electrodynamics

In a Classical Field Theory, such as Classical Electrodynamics, we can inves-
tigate the properties of the electromagnetic field by considering the effect of a
set of well localized external sources. These can be *electric charges* or, more
generally, some well defined distribution of *electric currents.* The result is fa-
miliar to us: the external currents set up a radiation field which propagates in
space, a propagating electromagnetic field. In Maxwell's electrodynamics these
effects are described by Maxwell's equations, *i.e.,* the equations of motion of
the electromagnetic field in the presence of a current distribution $j^\mu(x)$

$$\partial^2 \, A^\mu(x) = j^\mu(x) \tag{1}$$

where we have assumed the Lorentz gauge condition $(\partial_\mu A^\mu = 0)$, *i.e.,* the wave
equation.

In Classical Electrodynamics the solutions to this equation is found by using
of the *Green Function* $G(x, x')$,

$$\partial_x^2 G(x, x') = \delta^4(x - x') \tag{2}$$

which satisfies the *boundary condition* that

$$G(x, x') = 0 \quad \text{if} \quad x_0 < x_0' \tag{3}$$

1

This is the *retarded Green Function*, and it vanishes for events in the past (*i.e.*, for $x_0 < x_0'$).

The wave equations in the presence of a set of currents $j^\mu(x)$ is an inhomogeneous partial differential equation (p. d. e.). For times in the remote past (*i.e.*, before any currents were present) there should be no electromagnetic field present. The choice of retarded boundary conditions guarantees that the system be *causal*. The solution to the inhomogeneous p.d.e. is, as usual, the sum of an *arbitrary* solution of the homogenous equation, A_{in}^μ, which represents a pre-existing electromagnetic field, and a *particular* solution of the inhomogeneous field equation. We write the general solution in the form

$$A^\mu(x) = A_{in}^\mu(x) + \int d^4x' G_R(x - x') j^\mu(x') \tag{4}$$

where $A_{in}^\mu(x)$ is a solution of the wave equation in free space (in the absence of sources),

$$\partial^2 A_{in}^\mu(x) = 0 \tag{5}$$

Thus, all we need to know is the Green Function. Notice that the choice of retarded boundary conditions insures that, for $x_0 < x_0'$, $A^\mu(x) = A_{in}^\mu(x)$, since $G_R(x - x') = 0$ for $x_0 < x_0'$.

Let us solve for the Green Function $G(x, x')$. This is most easily done by considering the Fourier transform of $G(x, x')$

$$G(x, x') = \int \frac{d^4p}{(2\pi)^4} e^{ip \cdot (x - x')} \widetilde{G}(p) \tag{6}$$

where $p \equiv p^\mu$ and $p \cdot x \equiv p_0 x_0 - \vec{p} \cdot \vec{x}$. It is easy to check that the Fourier transform $\widetilde{G}(p)$ should be given by

$$\widetilde{G}(p) = -\frac{1}{p^2} \tag{7}$$

But we have two problems now. First, $\widetilde{G}(p)$ has a singularity at $p^2 \equiv p_0^2 - \vec{p}^2 = 0$, *i.e.*, at the eigenfrequencies of the normal modes of the free electromagnetic field $p_0 = \pm|\vec{p}|$. Thus the integral is ill-defined and some definition must be given about what to do with the singularity. Second, this $G(x, x')$ does not satisfy (at least not in any obvious way) the boundary conditions. We will solve both problems simultaneously. Let us define the *Retarded Green Function* by

$$G_R(x, x') \equiv \Theta(x_0 - x_0') G(x, x') \tag{8}$$

where

$$\Theta(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases} \tag{9}$$

Therefore, $G_R(x, x')$ vanishes for $x_0 < x_0'$ and is equal to $G(x - x')$ for $x_0 > x_0'$. The step (Heaviside) function $\Theta(x)$ has the formal integral representation (a Fourier transform)

$$\Theta(x) = \lim_{\epsilon \to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega \frac{e^{i\omega x}}{\omega - i\epsilon} \tag{10}$$

2

where the integral is interpreted as a *contour integral* over the contours of Fig. 1. Thus, when closing the contour as in the case $x < 0$, the contour does not
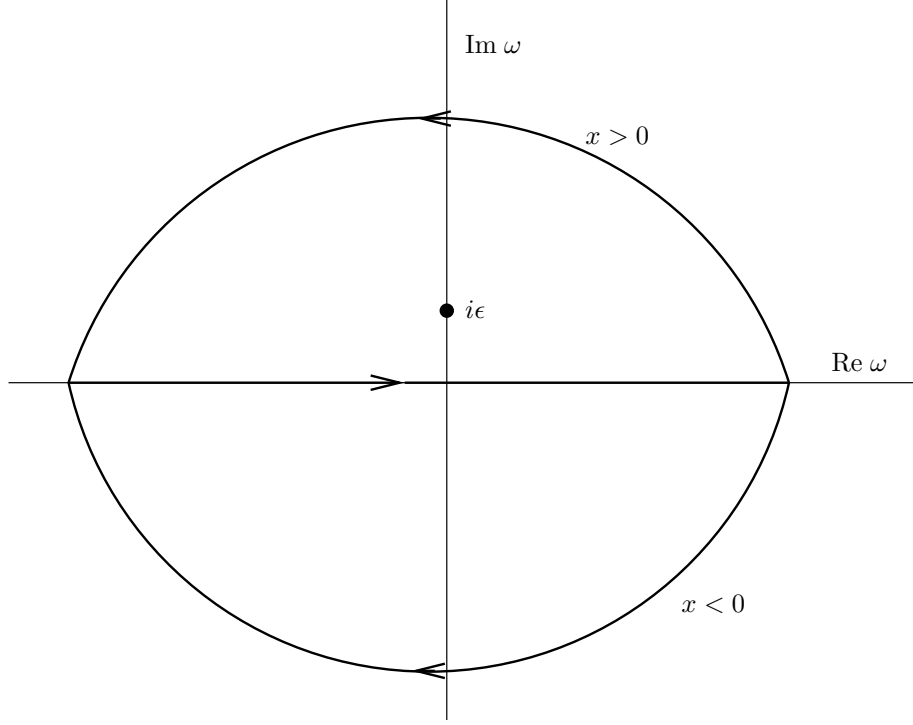

Figure 1: Contour in the complex plane that defines the function $\Theta(x)$.

contain the pole and the integral vanishes. Conversely, for $x > 0$, we close the contour on a large arc in the upper half plane and pick up a contribution from the enclosed pole equal to the residue, $e^{-\epsilon x}$ which converges to 1 as $\epsilon \to 0^+$. Notice that the integral on the large arc in the upper half plane converges to zero (for arcs with radius $R \to \infty$) only if $x > 0$.

We define the retarded Green function $G_R(x - x')$ by the following expression,

$$G_R(x - x') = -i \lim_{\epsilon \to 0^+} \int \frac{d^4p}{(2\pi)^4} \frac{e^{-ip \cdot (x - x')}}{(p_0 + i\epsilon)^2 - \vec{p}^{\,2}} \qquad (11)$$

which satisfies all of the requirements. We can also define the *advanced Green* function $G_A(x - x')$ which vanishes in the future, but not in the past,

$$G_A(x - x') = 0 \qquad x_0 - x'_0 > 0 \qquad (12)$$

by changing the sign of ϵ, *i.e.,*

$$G_A(x - x') = -i \lim_{\epsilon \to 0^+} \int \frac{d^4p}{(2\pi)^4} \frac{e^{-ip \cdot (x - x')}}{(p_0 - i\epsilon)^2 - \vec{p}^{\,2}} \qquad (13)$$
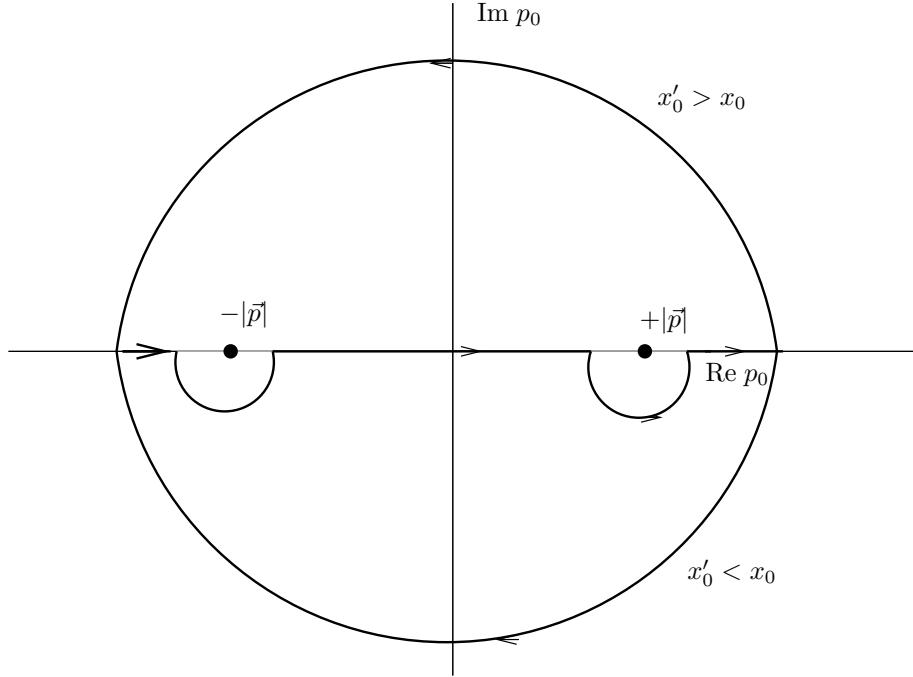
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Figure 2: Contour in the complex plane that defines retarded Green function.

Now the poles are on the upper half-plane and we get zero for $x'_0 - x_0 > 0$ but we pick up the poles for $x'_0 - x_0 < 0$ when we close on the lower half plane.

There are still two other possible choices of contours, such as the one shown in figure 3. In this case, when we close on the contour γ^+ in the upper-half plane, we pick up the pole at $-|\vec{p}|$ and the resulting frequency integral is

$$\oint_{\gamma^+} \frac{dp_0}{2\pi i} \frac{e^{-ip \cdot (x - x')}}{p_0^2 - \vec{p}^2} = \frac{e^{i\vec{p} \cdot (\vec{x} - \vec{x}') + i|\vec{p}|(x_0 - x'_0)}}{2(-|\vec{p}|)} \qquad x_0 < x'_0 \qquad (14)$$

while in the opposite case we get

$$\oint_{\gamma^-} \frac{dp_0}{2\pi i} \frac{e^{-ip \cdot (x - x')}}{p_0^2 - \vec{p}^2} = -\frac{e^{i\vec{p} \cdot (\vec{x} - \vec{x}') - i|\vec{p}|(x_0 - x'_0)}}{2|\vec{p}|} \qquad x_0 > x'_0 \qquad (15)$$

Thus, this choice the contour yields the Green function

$$G_F(x - x') = -\int \frac{d^3 p}{(2\pi)^3 2|\vec{p}|} \quad \left\{ \Theta(x'_0 - x_0) \, e^{-i|\vec{p}|(x'_0 - x_0) + i\vec{p} \cdot (\vec{x} - \vec{x}')} \right.$$
$$\left. + \Theta(x_0 - x'_0) e^{+i|\vec{p}|(x'_0 - x_0) - i\vec{p} \cdot (\vec{x} - \vec{x}')} \right\}$$
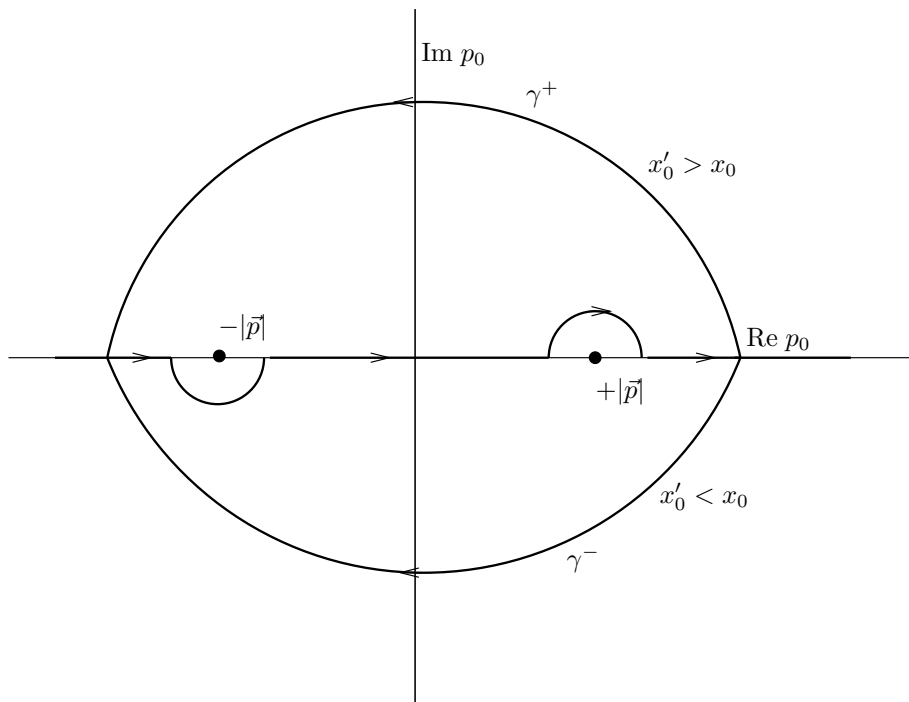$$(16)$$

4

Figure 3: Contour in the complex plane that defines Feynman propagator, or time ordered Green function.

which is known as the *Feynman Green function* and it bears a close formal resemblance to the mode expansions of free field theory. We will see below that there is indeed a reason for that. Notice that, in Maxwell's theory the zero component for the 4-momentum p_0 is equal to $|\vec{p}|$, and that the integration measure is Lorentz invariant. Also notice that this Feynman *propagator* or *Green function* propagates the *positive frequency* modes *forward* in time and the *negative frequency* modes backward in time. The alternative choice of contour simply yields the negative of $G_F(x - x')$.

10.2 The Propagator in Non-relativistic Quantum Mechanics

In non-relativistic quantum mechanics, the motion of quantum states is governed by the Schrödinger Equation

$$(i\hbar\partial_t - H)\psi = 0 \tag{17}$$

where $H = H_0 + V$. Let V be some position and time-dependent potential which vanishes (*very slowly*) both in the remote past ($t \to -\infty$) and in the

remote future ($t \to +\infty$). In this case, the eigenstates of the system are, in both limits, eigenstates of H_0. If $V(x,t)$ varies slowly with time, the states of H evolve smoothly, or adiabatically. Thus, we are describing *scattering processes* between free particle states Let $F(x't'|xt)$ denote the amplitude
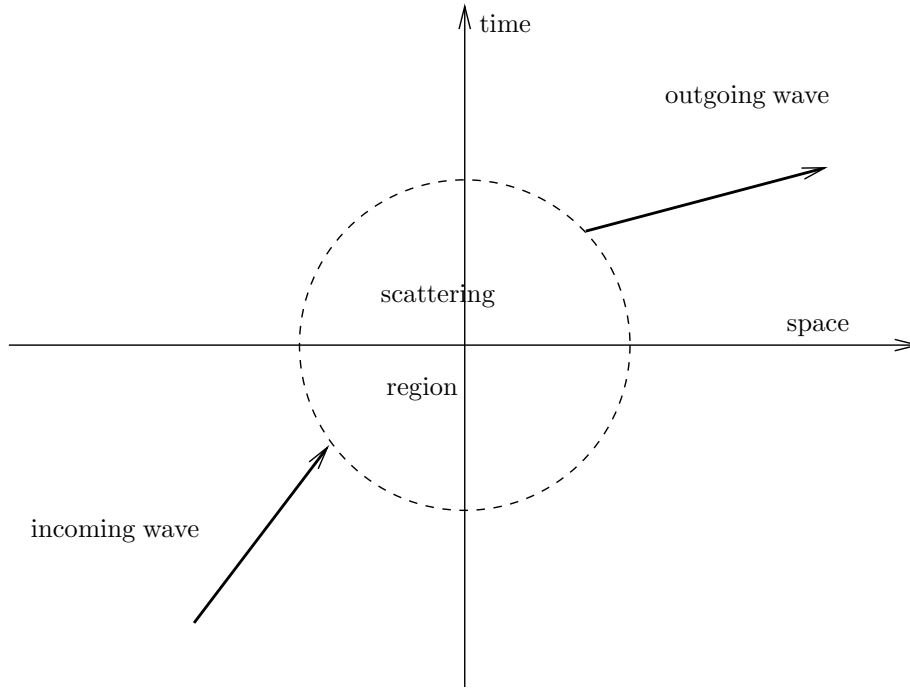

Figure 4: A scattering process.

$$F(x't'|xt) \equiv \langle x't'|xt \rangle \tag{18}$$

We have already introduced this amplitude when we discussed the path integral picture of Quantum Mechanics.

Let us suppose that at some time t the system has is in the state $|\psi(t)\rangle = |xt\rangle$. At some time $t' > t$, the state of the system is $|\psi, t'\rangle$ which is obtained by solving the Schrödinger equation

$$i\hbar \partial_t |\psi\rangle = H|\psi\rangle \tag{19}$$

where H is, in general, time-dependent. The formal solution of this equation is

$$|\psi(t')\rangle = T \, e^{-\dfrac{i}{\hbar} \int_t^{t'} dt'' H(t'')} \, |\psi(t)\rangle \tag{20}$$

where T is the time ordering symbol, *i.e.,*

$$T e^{\frac{-i}{\hbar} \int_t^{t'} dt'' H(t'')} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i}{\hbar} \right)^n \int_t^{t'} dt_1 \dots \int_t^{t_{n-1}} dt_n H(t_1) \dots H(t_n) \tag{21}$$

Thus, the amplitude $F(x't'|xt)$ is

$$F(x't'|xt) = \langle x't'|xt \rangle \equiv \langle x'|\psi(t') \rangle \tag{22}$$

Hence, if the initial state $|\psi(t)\rangle$ is $|\psi(t)\rangle = |x\rangle$ we get

$$F(x't'|xt) = \langle x'| T e^{-\frac{i}{\hbar} \int_t^{t'} dt'' H(t'')} |x\rangle \tag{23}$$

For the case of an *arbitrary* initial state $|\psi(t)\rangle$ we get

$$\langle x'|\psi(t') \rangle = \langle x'| e^{-\frac{i}{\hbar} \int_t^{t'} dt'' H(t'')} |\psi(t)\rangle \tag{24}$$

Since the states $\{|x>\}$ are complete, we have the completeness relation

$$1 = \int dx |x\rangle \langle x| \tag{25}$$

which allows us to write

$$\langle x'|\psi(t') \rangle = \int_{-\infty}^{+\infty} dx' \langle x'| e^{-\frac{i}{\hbar} \int_t^{t'} dt'' H(t'')} |x\rangle \langle x|\psi(t)\rangle \tag{26}$$

so, we get

$$\psi(x', t') = \int_{-\infty}^{+\infty} dx' \langle x't'|xt \rangle \psi(x, t) \tag{27}$$

In other words, the amplitude $F(x't', xt)$ is the kernel of the time evolution for arbitrary states. The amplitude $F(x't'|xt)$ is known as the *Schwinger function.*

The initial state $|\psi(t)\rangle$ and the final state $|\psi(t')\rangle$ are connected by the *evolution operator* $U(t', t)$

$$U(t', t) \equiv T e^{-\frac{i}{\hbar} \int_t^{t'} dt'' H(t'')} \tag{28}$$

which is *unitary* since, as a result of the Hermiticity of the Hamiltonian, we have

$$\begin{aligned} U^\dagger(t', t) &= T e^{\frac{i}{\hbar} \int_t^{t'} dt'' H(t'')} \\ &= T e^{-\frac{i}{\hbar} \int_{t'}^{t} dt'' H(t'')} = U(t, t') \end{aligned} \tag{29}$$

Be definition $U(t, t')$ is the *inverse* of $U(t', t)$ since it involves the states *backwards* in time. In addition, the operator $U(t', t)$ obeys the initial condition

$$\lim_{t' \to t} U(t', t) = I \tag{30}$$

where I is the identity operator. If the Hamiltonian is time-independent, the evolution operator is

$$U(t', t) = T \, e^{-\frac{i}{\hbar} \int_t^{t'} dt'' H(t'')} = e^{-\frac{i}{\hbar} H(t' - t)} \tag{31}$$

These ideas will also allow us to introduce the *Scattering Matrix* (or *S-Matrix*). If $\psi_i(x, t)$ is some initial state and $\psi_f(x', t')$ is some final state, the matrix elements of the S-matrix between states ψ_i and ψ_f, S_{fi} are obtained by evolving the state ψ_i up to time t' and projecting it onto the state ψ_f. Namely

$$S_{fi} = \lim_{t' \to +\infty} \lim_{t \to -\infty} \int dx \int dx' \psi_f^*(x't') \langle x't' | xt \rangle \psi_i(x, t) \tag{32}$$

Let us define the *Green function* or *propagator* $G(x't' | xt)$

$$G(x't' | xt) \equiv -\frac{i}{\hbar} \Theta(t' - t) \langle x't' | xt \rangle = \frac{-i}{\hbar} \Theta(t' - t) F(xt' | xt) \tag{33}$$

It satisfies the equation

$$(i\hbar \partial_{t'} - H(x')) \, G(x't' | xt) = \delta(x - x')\delta(t - t') \tag{34}$$

with the boundary condition

$$G(x't' | xt) = 0 \qquad \text{if} \qquad t' < t \tag{35}$$

Hence $G(x't' | xt)$ is the *retarded propagator*.

In terms of G, the S-matrix is given by (recall that $t' > t$)

$$S_{fi} = i \lim_{t' \to +\infty} \lim_{t \to -\infty} \int dx \int dx' \psi_f^*(x', t') G(x't' | xt) \psi_i(x, t) \tag{36}$$

Let us consider now the case of a free particle with Hamiltonian H_0 which is coupled to an external perturbation represented by a potential $V(x, t)$. The free Green function, G_0, satisfies the equation

$$(i\hbar \partial_{t'} - H_0(x')) \, G_0 = \delta(x' - x)\delta(t' - t) \tag{37}$$

G_0 can be regarded as the matrix elements of the following operator

$$G_0(x't' | xt) = \langle x't' | (i\hbar \partial_t - H)^{-1} | xt \rangle \tag{38}$$

Clearly, G satisfies the same equation but with the full H, *i.e.,*

$$(i\hbar \partial_{t'} - H(x')) \, G = 1 \tag{39}$$

8

Hence, we can write
$$[(i\hbar\partial_{t'} - H_0) - V]\, G = 1 \tag{40}$$
By using the definition of G_0, we get the operator equation
$$(G_0^{-1} - V)G = 1 \tag{41}$$
Thus, G satisfies the integral equation
$$G(x't', xt) = G_0(x't'|xt) + \int dx'' \int dt'' G_0(x't'|x't'')V(x't'')G(x't''|xt) \tag{42}$$
which is known as the *Dyson Equation*. It has the formal operator solution
$$G^{-1} = G_0^{-1} - V \tag{43}$$
The integral equation can also be solved by iteration, which amounts to a perturbative expansion expansion in powers of V. The result is the *Born series*. Using an obvious matrix notation we get
$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \ldots \tag{44}$$
We will represent this series by a set of *diagrams*. Let us consider the first term to which we assign the diagram of figure 5. The oriented arrow ranging from
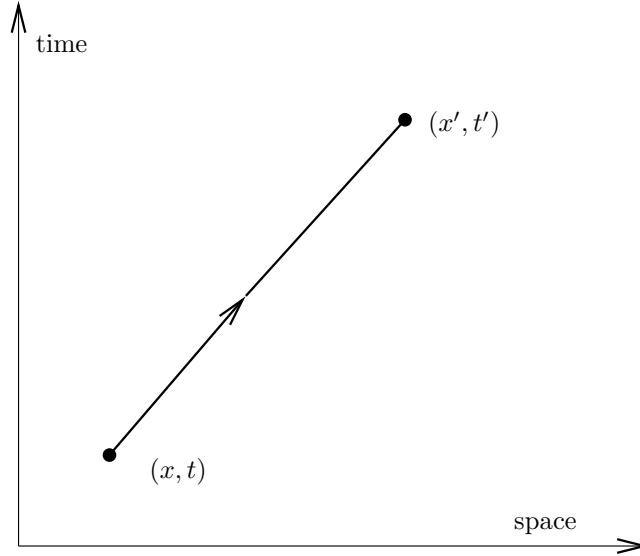

Figure 5: The zeroth order term.

(xt) to $(x't')$ represents the unperturbed propagator $G_0(x't'|xt)$. Because of

the causal boundary conditions obeyed by G_0 it can only propagate forward in time. The second term, of the series, the *Born approximation*, $\delta G^{(1)}$

$$\delta G^{(1)}(x't'|xt) = \int dx' \int dt'' G_0(x't'|x''t'')V(x''t'')G_0(x''t''|xt) \qquad (45)$$

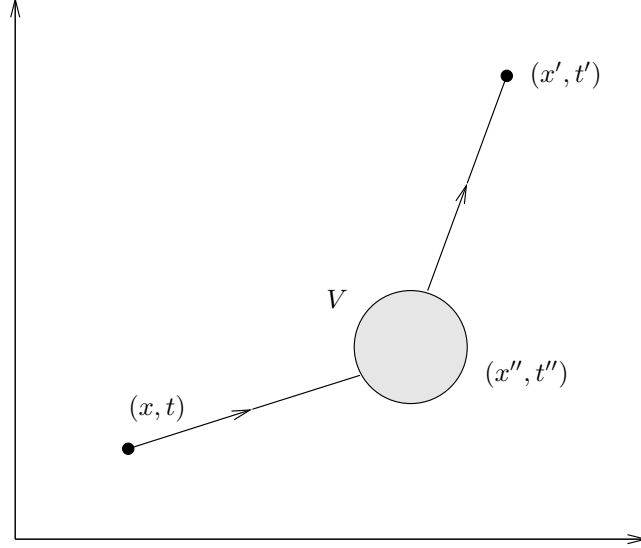is represented by the diagram where the "blob" represents the action of the

Figure 6: The first order term: the Born Approximation.

potential V. In general we get a diagram of the form which represents a multiple scattering process. Notice that all the contributions propagate strictly forward in time.

Let us compute the propagator $G_0(x't'|xt)$ for a free spinless particle in three-dimensional space. The Hamiltonian H is just, $H = -\frac{\hbar^2}{2m}\nabla^2$. Thus, G_0 obeys the equation

$$(i\hbar\partial_{t'} + \frac{\hbar^2}{2m}\nabla_x^2)G_0(x't'|xt) = \delta^3(x'-x)\delta(t'-t) \qquad (46)$$

we *causal* boundary conditions, $G(x't'|xt) = 0$ (if $t' < t$). Given the symmetries of this very simple system we can Fourier expand G_0.

$$G_0(x't'|xt) = \int \frac{d^3p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \widetilde{G}_0(\vec{p}, \omega)e^{\frac{i}{\hbar}\vec{p}\cdot(\vec{x}'-\vec{x})-i\omega(t'-t)} \qquad (47)$$

By direct substitution we find that $\widetilde{G}_0(\vec{p}, \omega)$ must be given by

$$\widetilde{G}_0(\vec{p}, \omega) = \frac{1}{\hbar\omega - \frac{\vec{p}^{\,2}}{2m}} \qquad (48)$$
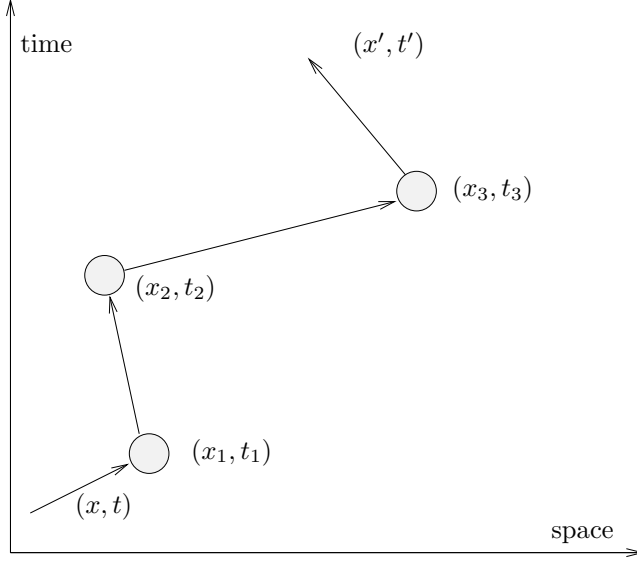
10

Figure 7: Multiple scattering processes.

Notice that, once again, $\widetilde{G}_0(\vec{p}, \omega)$ has a pole at $\hbar\omega = \dfrac{\vec{p}^{\,2}}{2m}$ which is the dispersion law (*i.e.*, , the "mass shell"). Apart from being singular, this "solution" does not obey the causal boundary condition. We will enforce the boundary condition by deforming the integration contour in the complex *frequency* plane. Following our previous discussion on the Green function for classical electrodynamics we simply move the pole by an infinitesimal positive amount ϵ into the upper half-complex frequency plane. We write the *retarded* propagator as

$$G_0^{ret}(\vec{p}, \omega) = \frac{1}{\hbar\omega - \dfrac{\vec{p}^{\,2}}{2m} + i\epsilon} \tag{49}$$

and we will take the limit $\epsilon \to 0^+$ at the end of our calculations. Thus the frequency integral is equal to

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega(t'-t)}}{\hbar\omega - \dfrac{\vec{p}^{\,2}}{2m} + i\epsilon} = -\frac{i}{\hbar}\Theta(t'-t)e^{-\frac{i}{\hbar}\frac{\vec{p}^{\,2}}{2m}(t'-t)} \tag{50}$$

Hence the full Green function $G_0(x't'|xt)$ is

$$G_0(x't'|xt) = -\frac{i}{\hbar}\Theta(t'-t)\int \frac{d^3p}{(2\pi)^3} e^{-\frac{i}{\hbar}\frac{\vec{p}^{\,2}}{2m}(t'-t) + \frac{i}{\hbar}\vec{p}\cdot(\vec{x}'-\vec{x})} \tag{51}$$

11

Let $\psi_{\vec{p}}(xt)$ denote the wave functions for the *stationary states* $|\vec{p}\rangle$, *i.e.*,

$$\psi_{\vec{p}}(x,t) = \frac{1}{(2\pi)^{3/2}} e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{x} + \frac{i}{\hbar}E(\vec{p})t} \tag{52}$$

where $E(\vec{p}) = \dfrac{\vec{p}^2}{2m}$. We see that $G_0(x't'|xt)$ can be written in the form

$$G_0(x't'|xt) = -\frac{i}{\hbar}\,\Theta(t'-t)\int d^3p\,\psi_{\vec{p}}(x't')\psi_{\vec{p}}^*(xt) \tag{53}$$

In general, if the Hamiltonian has a complete set of stationary states $\{|n\rangle\}$ with wave functions $\psi_n(x)$ and eigenvalues E_n, the Green function is

$$G_0^{\mathrm{ret}}(x't'|xt) = -\frac{i}{\hbar}\Theta(t'-t)\sum_n \psi_n(x't')\psi_n^*(xt) \tag{54}$$

where

$$\psi_n(xt) = \psi_n(x)e^{-\frac{i}{\hbar}E_n t} \tag{55}$$

If the system is isolated, the Hamiltonian is time-independent and the Green function is a function of $t - t'$. In this case it is convenient to consider the Fourier transform

$$G_0^{\mathrm{ret}}(x';x|t'-t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,G_0^{\mathrm{ret}}(x',x;\omega)\,e^{i\omega(t-t')/\hbar} \tag{56}$$

where we have to pick the correct integration contour so that G_0^{ret} is retarded.

Quite explicitly we find

$$G_0^{\mathrm{ret}}(x';x|\omega) = \frac{1}{\hbar}\lim_{\epsilon\to 0^+}\sum_n \frac{\psi_n(x')\psi_n^*(x)}{\omega - \frac{E_n}{\hbar} + i\epsilon} \tag{57}$$

The denominators in this equation have zeros on the real frequency axis as $\epsilon \to 0^+$. Thus, the Green function is a series of *distributions*. In the limit $\epsilon \to 0^+$ we can write

$$\lim_{\epsilon\to 0^+}\frac{1}{x+i\epsilon} = \mathcal{P}\frac{1}{x} - i\pi\delta(x) \tag{58}$$

where where $\mathcal{P}$ denotes the principal value and $\delta(x)$ is the Dirac delta function. Hence we can write the following expressions for the real and imaginary parts of the Green function

$$
\begin{aligned}
\mathrm{Re}\,G_0^{\mathrm{ret}}(x';x|\omega) &= \sum_n \mathcal{P}\frac{\psi_n(x')\psi_n^*(x)}{\hbar\omega - E_n}\\
\mathrm{Im}\,G_0^{\mathrm{ret}}(x';x|\omega) &= -\pi\sum_n \psi_n(x')\psi_n^*(x)\delta(\hbar\omega - E_n)
\end{aligned}
\tag{59}
$$

12

We can use these results to find an expression for the *density of states* $\rho(\omega)$

$$\rho(\omega) = \sum_n \delta(\hbar\omega - E_n) \tag{60}$$

in terms of the retarded Green function of the form

$$\rho(\omega) = -\frac{1}{\pi}\text{Im} \int dx \, G_0^{\text{ret}}(x; x|\omega) \tag{61}$$

In other words, the spectral density is determined by the imaginary part of the Green function. Below we will find similar relationships for other quantities of physical interest.

Let us close by noting that there is a close connection between the Green function in Quantum Mechanics and the kernel of the diffusion equation. In d-dimensional space the Green function is

$$G_0(\vec{x}', t'|\vec{x}, t) = -\frac{i}{\hbar}\Theta(t' - t) \int \frac{d^d p}{(2\pi)^d} e^{-\frac{i}{\hbar}\frac{\vec{p}^2}{2m}(t' - t) + \frac{i}{\hbar}\vec{p}\cdot(\vec{x}' - \vec{x})} \tag{62}$$

By completing squares inside the exponent

$$\begin{aligned}
\frac{\vec{p}^2}{2m}(t' - t) - \vec{p}\cdot(\vec{x}' - \vec{x}) &= \frac{(t' - t)}{2m}\left[\vec{p} - 2m\vec{p}\cdot\frac{\vec{x}' - \vec{x}}{(t' - t)}\right] \\
&= \left(\frac{t' - t}{2m}\right)\left[\vec{p} - \left(\frac{\vec{x}' - \vec{x}}{t' - t}\right)m\right]^2 - \frac{m|\vec{x}' - \vec{x}|^2}{2|t' - t|}
\end{aligned} \tag{63}$$

we can write

$$\begin{aligned}
G_0(\vec{x}', t'|\vec{x}, t) = \\
-\frac{i}{\hbar}\Theta(t' - t) \int \frac{d^d p}{(2\pi)^d} \, e^{-\frac{i}{\hbar}\left(\frac{t' - t}{2m}\right)\left(\vec{p} - \left(\frac{\vec{x}' - \vec{x}}{t' - t}\right)m\right)^2 + \frac{i}{2\hbar}m\frac{|\vec{x}' - \vec{x}|^2}{|t' - t|}}
\end{aligned} \tag{64}$$

After a straightforward integration, we find that G_0 is equal to

$$G_0(\vec{x}', t'|\vec{x}, t) = -\frac{i}{\hbar}\Theta(t' - t) \left(\frac{m\hbar}{2\pi(t' - t)}\right)^{d/2} e^{\frac{im}{2\hbar}\frac{|\vec{x}' - \vec{x}|^2}{(t' - t)}} \tag{65}$$

This formula is strongly reminiscent of the Kernel for the Heat Equation (or Diffusion Equation)

$$\partial_\tau \psi = D \, \nabla^2 \, \psi \tag{66}$$

where D is the diffusion constant and τ is the diffusion time. Indeed, after an analytic continuation to *imaginary time*, $t \to i\tau$, the Schrödinger equation

13

becomes a diffusion equation with a diffusion constant $D = \frac{\hbar}{2m}$. The Green function (or *Heat Kernel*) for the Heat equation is

$$K(\vec{x}'\tau'|\vec{x}\tau) = \Theta(\tau' - \tau)\frac{1}{(4\pi D\tau)^{d/2}} \; e^{-\frac{|\vec{x}' - \vec{x}|^2}{4D(\tau' - \tau)}} \qquad (67)$$

which, of course, agrees with G_0. This connection between quantum mechanics and diffusion processes is central to the path-integral picture of quantum mechanics.

10.2.1 Analytic Properties of the Propagator of the Relativistic Real Scalar Field and of the Dirac Field

The propagator for a free real relativistic field $G_0(x, x') = -i\langle 0|T\phi(x)\phi(x')|0\rangle$ is the solution of the partial differential equation

$$(\partial^2 + m_0^2)\, G_0(x, x') = \delta^4(x - x') \qquad (68)$$

which we have discussed and solved before. $G_0(x, x')$ can be calculated by the usual Fourier expansion methods,*i.e.*,

$$G_0(x, x') = \int \frac{d^4p}{(2\pi)^4} \; \widetilde{G}_0(p) \; e^{+ip\cdot(x - x')} \qquad (69)$$

where $\widetilde{G}_0(p)$ is given by

$$\widetilde{G}_0(p) = \frac{-1}{p^2 - m^2} \qquad (70)$$

where $p^2 = p_\mu p^\mu$. Once again, we will have to give a prescription for going around the poles of $\widetilde{G}_0(p)$ which yields the correct boundary conditions. The poles of $\widetilde{G}_0(p)$ are located at $p_0 = \pm\sqrt{\vec{p}^2 + m^2} \mp i\epsilon$. We will use the integration paths shown in figure 8. On the integration path γ^+ we find the result

$$-\oint_{\gamma^+} \frac{dp_0}{2\pi} \frac{e^{+ip_0(x_0 - x_0')}}{p_0^2 - (\vec{p}^2 + m^2) + i\epsilon} \xrightarrow[\epsilon \to 0^+]{} i\frac{e^{-i\sqrt{\vec{p}^2 + m^2}\,(x_0 - x_0')}}{2\sqrt{\vec{p}^2 + m^2}} \qquad (71)$$

provided $x_0 > x_0'$. Similarly, on γ^- we get

$$-\oint_{\gamma^-} \frac{dp_0}{2\pi} \frac{e^{ip_0(x_0 - x_0')}}{p_0^2 - (\vec{p}^2 + m^2) + i\epsilon} \xrightarrow[\epsilon \to 0^+]{} i\frac{e^{i\sqrt{\vec{p}^2 + m^2}(x_0 - x_0')}}{2\sqrt{\vec{p}^2 + m_0^2}} \qquad (72)$$

provided $x_0 < x_0'$. By collecting terms we get

$$\begin{aligned} G_0(x, x') &= i\Theta(x_0 - x_0') \int \frac{d^3p}{(2\pi)^3 2\omega(\vec{p})} e^{+i\vec{p}\cdot(\vec{x} - \vec{x}') - i\omega(\vec{p})(x_0 - x_0')} \\ &+ i\Theta(x_0' - x_0) \int \frac{d^3p}{(2\pi)^3 2\omega(\vec{p})} e^{-i\vec{p}\cdot(\vec{x} - \vec{x}') + i\omega(\vec{p})(x_0 - x_0')} \end{aligned}$$
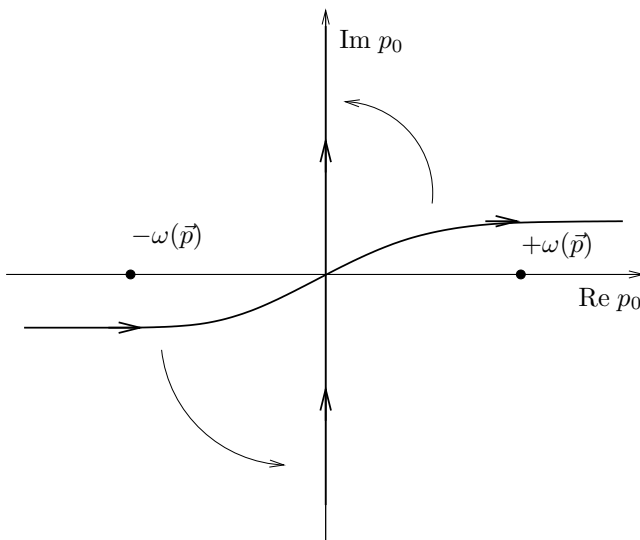
$$(73)$$

14

Figure 8: Wick Rotation.

This formula shows that $G_0(x, x')$ does satisfy the required boundary condition. It also shows that the positive frequency components of the field propagate forwards in time while the negative frequency components propagate backwards in time.

The simplest way to compute $G_0(x, x')$ is by means of an analytic continuation (or Wick rotation) to imaginary time, $x_0 \to i x_4$. This amounts to a rotation of the integration contour from the *real* p_0 axis to the *imaginary* p_0 axis, namely $p_0 \to i p_4$. The Wick-rotated or Euclidean Green function $G_0^E(x, x')$, *i.e.,* the Euclidean propagator that we calculated before, is given by

$$G_0(x, x') = i \int \frac{d^4 p}{(2\pi)^4} \frac{e^{-ip(x_0 - x_0')}}{p^2 + m^2} \equiv i G_0^E(x, x') \tag{74}$$

where $p^2 = -\sum_{i=1}^{4} p_i p_i$ and $p \cdot x = -\sum_{i=1}^{4} p_i x_i$.

The time-ordered, or Feynman, propagator does not obey causality since it does not vanish for space-like separated events ($s^2 < 0$). We can define a *causal*, or *retarded*, propagator which obeys the causal boundary condition $G(x, x') = 0$ except inside the *forward* light-cone. Similarly, it is also possible to define an *advanced*, or anti-causal, propagator which vanishes outside the *backward* light-cone. We will discuss only the retarded propagator $G_{\text{ret}}(x - x')$.

The retarded propagator is defined by computing the frequency integral on the path shown in the figure 9, $G_{\text{ret}}(x - x')$ is given by
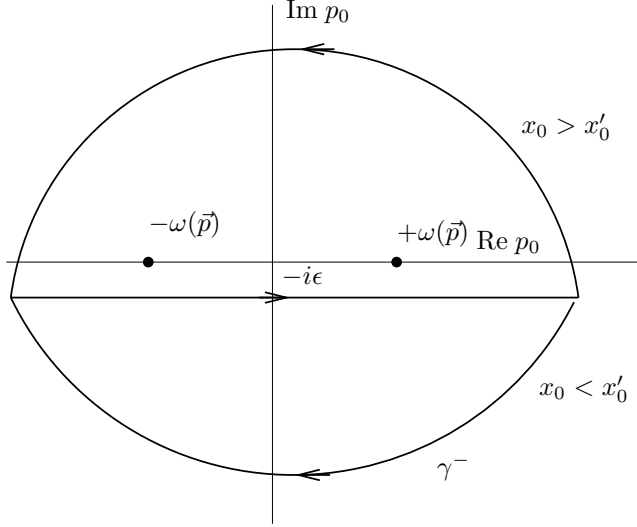
Figure 9: Integration path for the retarded Green function.

$$
\begin{aligned}
G_{\text{ret}}(x - x') &= -\int \frac{d^3p}{(2\pi)^3} e^{-i\vec{p} \cdot (\vec{x} - \vec{x}')} \int_{-\infty}^{+\infty} \frac{dp_0}{2\pi} \frac{e^{ip_0(x_0 - x_0')}}{p_0^2 - \omega^2(\vec{p})} \\
&\equiv -i \int \frac{d^3p}{(2\pi)^3 2\omega(\vec{p})} e^{-i\vec{p} \cdot (\vec{x} - \vec{x}')} \int_{-\infty}^{+\infty} \frac{dp_0}{2\pi i} e^{ip_0(x_0 - x_0')} \\
&\qquad \times \left[\frac{1}{p_0 - \omega(\vec{p}) - i\epsilon} - \frac{1}{p_0 + \omega(\vec{p}) - i\epsilon} \right]
\end{aligned}
\tag{75}
$$

Hence, we get

$$
\begin{aligned}
G_{\text{ret}}(x - x') &= -i\Theta(x_0 - x_0') \\
\int \frac{d^3p}{(2\pi)^3 2\omega(\vec{p})} &\left[e^{i\omega(p)(x_0 - x_0') - i\vec{p} \cdot (\vec{x} - \vec{x}')} - e^{-i\omega(\vec{p})(x_0 - x_0') + i\vec{p} \cdot (\vec{x} - \vec{x}')} \right]
\end{aligned}
\tag{76}
$$

The integral over the momentum variables is just the quantity $i\Delta(x - x')$, that we have encountered before,

$$
i\Delta(x - x') = [\phi(x), \phi(x')] \equiv \langle 0 | [\phi(x), \phi(x')] | 0 \rangle
\tag{77}
$$

which allows us to write

$$
G_{\text{ret}}(x - x') = \Theta(x_0 - x_0')\Delta(x - x') = -i\Theta(x_0 - x_0')\langle 0 | [\phi(x), \phi(x')] | 0 \rangle
\tag{78}
$$

The same line of argument we have used here for the scalar field can be used for the Dirac field. The vacuum state of the Dirac theory is defined by filling

16

up all negative energy states. We now imagine that an external potential is adiabatically switched on and that, before that happened, there was an electron $e-$ propagating in the system. If the potential is not too strong, we can still describe its effects by means of a Born series of multiple scattering processes (Fig.10).
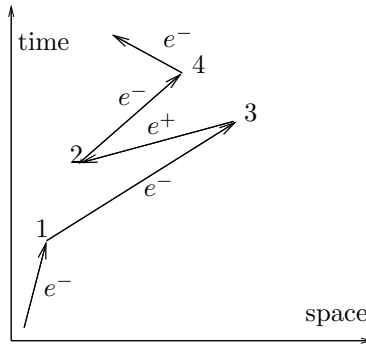
Figure 10: Scattering processes of a Dirac field.

The electron scatters off the potential at 1 and as a result it propagates up to 3. If the potential has the correct matrix elements, at 3 the positive energy solution may turn into a negative energy state. In general this won't be allowed since all negative energy states are filled up, unless a negative energy state got emptied (by the action of the potential) *before the electron became scattered into that state.* Indeed, the potential can *create a pair* out of the vacuum, *e.g.,* Fig.11:

Figure 11: Pair creation.

Thus, it can remove an electron from an occupied negative energy state and to promote it into a previously empty positive energy state. Hence, if the time t

lies between t_2 and t_3, there are *three* different states propagating in the system (Fig.12):

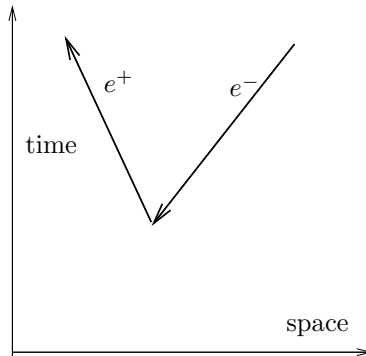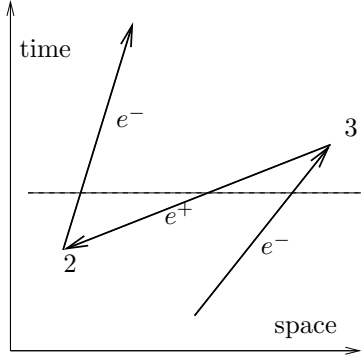

Figure 12: An intermediate state with an electron-positron pair.

1. a positive energy state which disappears at **3**

2. a negative energy state which propagates *backwards* in time from **3** to **2**

3. a positive energy state which appeared at **2**.

An alternative interpretation is that an electron-positron pair was created at **2** and that the positron annihilated with the original electron at **3**. This process clearly shows that the Dirac theory is a *quantum field theory*, and cannot be described within the framework of quantum mechanics with a fixed number of particles, as in the non-relativistic case. Thus, the Fock space description is essential to the relativistic case.

These arguments suggest that we may want to seek a propagator which propagates positive energy states forward in time while negative energy states propagate backwards in time. This is the Feynman, or time-ordered, propagator $S_F^{\alpha\alpha'}(x, x')$. It is straightforward to see that these requirements are met by

$$S_F^{\alpha\alpha'}(x, x') = -i\langle 0|T\psi_\alpha(x)\bar{\psi}_{\alpha'}(x')|0\rangle \tag{79}$$

which satisfies the equation of motion

$$(i\slashed{\partial} - m)S_F(x, x') = \delta^4(x - x') \tag{80}$$

The same methods that we used for the scalar field yield the answer (dropping the spinor indices)

$$S_F(x, x') = S_F(x - x') = \int \frac{d^4p}{(2\pi)^4} \frac{\slashed{p} + m}{p^2 - m^2 + i\epsilon} e^{-ip \cdot (x - x')} \tag{81}$$

18

where an $i\epsilon$ has been introduced in order to get the correct boundary conditions. We have also shown that $S_F(x - x')$ satisfies

$$S_F(x - x') = -(i\slashed{\partial} + m) \int \frac{d^4p}{(2\pi)^4} \frac{e^{-ip \cdot (x - x')}}{p^2 - m^2 + i\epsilon} = (i\slashed{\partial} + m)G_F(x - x') \quad (82)$$

where $G_F(x - x')$ is the Feynman or time-ordered propagator for a scalar field. The $i\epsilon$ prescription insures that positive energy states propagate forward in time while negative energy states propagate backward in time.

10.2.2   The Propagator for the Non-Relativistic Electron Gas

Let us now discuss the propagator, or *one-particle Green function*, for a non-relativistic free electron gas at finite density and zero temperature. It is defined in the usual way

$$G_0^{\alpha\alpha'}(x, x') = -i\langle \text{gnd}|T\psi_\alpha(x)\psi_{\alpha'}^\dagger(x')|\text{gnd}\rangle \quad (83)$$

where $\alpha\alpha'$ are spin indices. This propagator can be used to compute a number of quantities of physical interest. For example, the average *electron density* $\langle \hat{n}(x) \rangle$ is

$$\langle n(\vec{x}) \rangle = \langle \psi^\dagger(\vec{x})\psi(\vec{x}) \rangle = -i \lim_{\vec{x}' \to \vec{x}} \lim_{x_o' \to x_0} \text{tr } G(x, x') \quad (84)$$

Likewise the *current* $\langle \vec{j}(\vec{x}) \rangle$ is

$$\begin{aligned}
\langle \vec{j}(\vec{x}) \rangle &= \frac{\hbar}{2mi}\text{tr } \langle \psi^\dagger(x)\left(\vec{\nabla}_x\psi(x)\right) - \left(\vec{\nabla}_x\psi^\dagger(x)\right)\psi(x) \rangle \\
&= -\frac{1}{m} \lim_{\vec{x}' \to \vec{x}} \lim_{x_o' \to x_0} \left(\vec{\nabla}_{\vec{x}} - \vec{\nabla}_{\vec{x}'}\right) \text{tr } G(x, x')
\end{aligned}$$

$$(85)$$

and the *magnetization* $\vec{M}(x) = \langle \psi_\alpha^\dagger(x)\vec{\sigma}_{\alpha\beta}\psi_\beta(x) \rangle$,

$$\vec{M}(x) = -i \lim_{\vec{x}' \to \vec{x}} \lim_{x_o' \to x_0} \text{tr } [G(x, x)\vec{\sigma}] \quad (86)$$

Let us compute $G(x, x')$ by the standard method of Fourier transforms.

$$\begin{aligned}
G(x, x') &= \int \frac{d^3p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \; \widetilde{G}(\vec{p}, \omega) \; e^{i\,[\vec{p} \cdot (\vec{x} - \vec{x}') - \omega(t - t')]} \\
&\equiv \int \frac{d^4p}{(2\pi)^4} \; \widetilde{G}(p) \; e^{ip \cdot (x - x')}
\end{aligned}$$

$$(87)$$

where $p_0 = \omega$ and $t = x_0$. The field $\psi(x)$ can also be expanded ($\hbar = 1$)

$$\psi(x) = \int \frac{d^3p}{(2\pi)^3} \; \psi(\vec{p}) \; e^{i\,(\vec{p} \cdot \vec{x} - E(\vec{p})t)} \quad (88)$$

19

since $\psi(x)$ satisfies the equations of motion. Here $E(p)$ are the single particle energies, $E(p) = \frac{p^2}{2m} - \mu$. Thus, we get

$$
\begin{aligned}
G(x,t) &= -i \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3q}{(2\pi)^3} \Theta(t) \langle \text{gnd} | \psi(\text{p}) \psi^\dagger(\text{q}) | \text{gnd} \rangle e^{i \, (\vec{p} \cdot \vec{x} - E(\vec{p}) \, t)} \\
&+ i \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3q}{(2\pi)^3} \Theta(-t) \langle \text{gnd} | \psi^\dagger(\text{q}) \psi(\text{p}) | \text{gnd} \rangle e^{i \, (\vec{p} \cdot \vec{x} - E(\vec{p}) t)}
\end{aligned}
\tag{89}
$$

Recall that $|\text{gnd}\rangle$ is the state in which all negative energy states ($E(\vec{p}) < 0$ or $\epsilon(p) < \mu$) are filled. Thus

$$
G(x,t) = -i \int \frac{d^3p}{(2\pi)^3} \left[\Theta(t) \left(1 - n(\vec{p})\right) - \Theta(-t) n(\vec{p}) \right] e^{i \, (\vec{p} \cdot \vec{x} - E(\vec{p}) t)}
\tag{90}
$$

where $n(p)$ is the (zero-temperature) Fermi function

$$
n(\vec{p}) = \begin{cases} 1 & |\vec{p}| \le p_F \\ 0 & \text{otherwise} \end{cases}
\tag{91}
$$

Hence, we can write the Fourier transform $G(p,\omega)$ in the form

$$
G(p,\omega) = -i \left\{ \Theta(|\vec{p}| - p_F) \int_0^\infty e^{i(\omega - E(p))t} dt - \Theta(p_F - |\vec{p}|) \int_0^\infty dt \, e^{-i(\omega - E(p))t} \right\}
\tag{92}
$$

The integrals in this expression define distributions of the form

$$
\begin{aligned}
\int_0^\infty dt \, e^{ist} &= \lim_{\epsilon \to 0^+} \int_0^\infty dt \, e^{ist - \epsilon \, t} \\
&= i \lim_{\epsilon \to 0^+} \frac{1}{s + i\Delta} = i \left(\mathcal{P} \frac{1}{s} - i\pi \epsilon(s) \right)
\end{aligned}
\tag{93}
$$

where $\mathcal{P}\frac{1}{s}$ is the *principal value*

$$
\mathcal{P}\frac{1}{s} = \lim_{\epsilon \to 0} \frac{s}{s^2 + \epsilon^2}
\tag{94}
$$

and $\delta(s)$ is the Dirac δ-function.

We can use these results to write an expression for $\widetilde{G}_0(\vec{p}, \omega)$

$$
\widetilde{G}_0(\vec{p}, \omega) = \frac{\Theta(|\vec{p}| - p_F)}{\omega - E(\vec{p}) + i\epsilon} + \frac{\Theta(p_F - |\vec{p}|)}{\omega - E(\vec{p}) - i\epsilon}
\tag{95}
$$

where $E(\vec{p}) = \epsilon(\vec{p}) - \mu$. An equivalent (and more compact) expression is

$$
\widetilde{G}_0(\vec{p}, \omega) = \frac{1}{\omega - E(\vec{p}) + i\epsilon \, \text{sign}(|\vec{p}| - p_F)}
\tag{96}
$$

20

Notice that

$$
\begin{aligned}
\mathrm{Im}\widetilde{G}_0(\vec{p},\omega) &= -\pi\Theta(|\vec{p}|-p_F)\delta(\omega-\epsilon(\vec{p})+\mu)+\pi\Theta(p_F-|\vec{p}|)\delta(\omega-\epsilon(\vec{p})+\mu) \\
&= -\pi\delta(\omega-\epsilon(\vec{p})+\mu)\left[\Theta\left(|\vec{p}|-p_F\right)-\Theta(p_F-|\vec{p}|)\right]
\end{aligned}
\tag{97}
$$

The last identity shows that

$$
\mathrm{sign}\,\mathrm{Im}\widetilde{G}_0(\tilde{p},\omega)=-\mathrm{sign}\,\omega
\tag{98}
$$

Hence, we may also write $\widetilde{G}_0(p,\omega)$ as

$$
\widetilde{G}_0(\vec{p},\omega)=\frac{1}{\omega-E(\vec{p})+i\epsilon\,\mathrm{sign}\,\omega}
\tag{99}
$$

With this expression, we see that $\widetilde{G}_0(\vec{p},\omega)$ has poles at $\omega=E(\vec{p})$ and that all the poles with $\omega>0$ are infinitesimally shifted downwards to the lower half-plane, while the others are raised upwards to the upper half-plane by the same amount. Since $E(p)=\epsilon(p)-\mu$, all poles with $\epsilon(p)>\mu$ are shifted downwards, while all poles with $\epsilon(p)<\mu$ are shifted upwards.
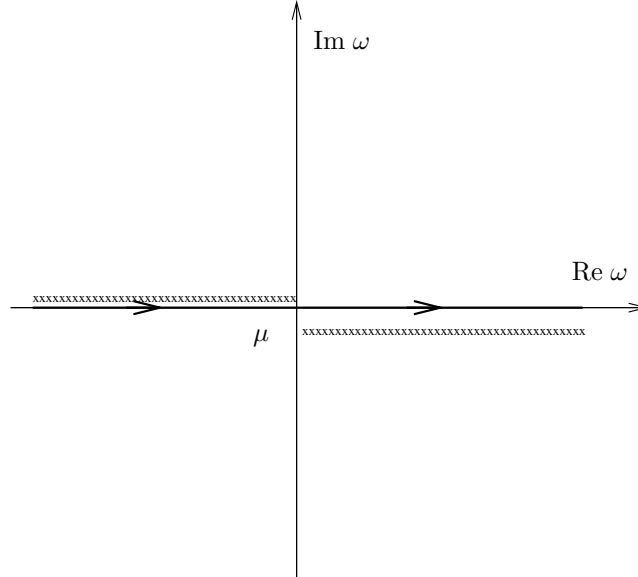

Figure 13: Analytic structure of the Green function at finite chemical potential μ.

10.3   The Scattering Matrix

The problems of real physical interest very rarely involve free fields. In general we have to deal with interacting fields. For the sake of definiteness we will consider a scalar field but the ideas that we will discuss have general applicability.

10.3.1   Interactions and the Interaction Representation

The field $\phi(\vec{x}, t)$ in the Heisenberg representation is related to the Schrödinger operator $\phi(\vec{x})$ through the time evolution generated by the equations of motion, *i.e.,*

$$\phi(\vec{x}, t) \equiv \phi(x) = e^{iHt} \phi(\vec{x}, 0) e^{-iHt} \tag{100}$$

(for $\hbar = 1$). Recall that in the Schrödinger representation the *fields are fixed* but the *states evolve* according to the Schrödinger equation

$$H|\Phi\rangle = i\partial_t|\Phi\rangle \tag{101}$$

Conversely, in the Heisenberg representation, the *states are fixed* but the *fields evolve* by following the equations of motion, *i.e.,*

$$i\partial_t\phi(x) = [\phi(x), H] \tag{102}$$

In an interacting system, the problem is precisely how to determine the evolution operator e^{iHt}. Thus, the Heisenberg representation cannot be constructed *a priori.*

Let us assume that the Hamiltonian can be split into a sum of two terms

$$H = H_0 + H_{int} \tag{103}$$

where H_0 represents a system whose states are fully known to us (*i.e.,* a problem that we know how to solve) and H_{int} represents the interactions. For technical reasons we will have to assume that $H_{int}(t)$, as a function of time, vanishes (very smoothly) both in the remote past and in the remote future. We now define the *Interaction Representation*. In the Interaction Representation, the *fields* ϕ_{in} evolve as free Heisenberg fields, *i.e.,*

$$i\partial_t\phi_{\text{in}}(x) = [\phi_{\text{in}}, H_0] \tag{104}$$

These operators create and destroy free *incoming* states (incoming since as $t \to -\infty$ there are no interactions). In the absence of interactions, the states would not evolve but, if interactions are present, they will. There is a unitary operator $U(t)$ which governs the time evolution of the states and the S-matrix.

We want to find an operator $U(t)$ such that

$$\phi(x, t) = U^{-1}\phi_{\text{in}}(x, t)U(t) \tag{105}$$

where $\phi(x, t)$ is the Heisenberg operator. The operator $U(t)$ must be *unitary* and satisfy the initial condition

$$\lim_{t \to -\infty} U(t) = I \tag{106}$$

22

Since $U(t)$ is unitary and invertible, it must satisfy the condition $U^{-1}(t) = U^\dagger(t)$. Thus

$$\frac{d}{dt}U(t)U^{-1}(t) + U(t)\frac{d}{dt}U^{-1}(t) = 0 \tag{107}$$

Since the operator ϕ_{in} obeys its equation of motion, we get

$$\begin{aligned}
\partial_t \phi_{\text{in}} &= \partial_t U \, \phi \, U^{-1} + U \, \partial_t \phi \, U^{-1} + U \, \phi \, \partial_t U^{-1} \\
&= \partial_t U \, \phi \, U^{-1} + iU \, [H, \phi] \, U^{-1} + U \, \phi \, U^{-1} \, U \, \partial_t U^{-1}
\end{aligned} \tag{108}$$

In other terms,

$$\partial_t \phi_{\text{in}} = iU(t)[H(\phi), \phi]U^{-1}(t) + \partial_t U U^{-1} \phi_{\text{in}} + \phi_{\text{in}} U \partial_t U^{-1} \tag{109}$$

Similarly, the Hamiltonian must obey the identity

$$H(\phi_{\text{in}}) = U(t)H(\phi)U^{-1}(t) \tag{110}$$

which implies that ϕ_{in} should obey

$$\partial_t \phi_{\text{in}} = i[H(\phi_{\text{in}}), \phi_{\text{in}}] + [(\partial_t U) \ U^{-1}, \phi_{\text{in}}] \tag{111}$$

Since ϕ_{in} obeys the free equation of motion, we find that the evolution operator $U(t)$ must satisfy the condition

$$i[H_{\text{int}}(\phi_{\text{in}}), \phi_{\text{in}}] + [\partial_t U \ U^{-1}, \phi_{\text{in}}] = 0 \tag{112}$$

Hence

$$[iH_{\text{int}}(\phi_{\text{in}}) + (\partial_t U) \ U^{-1}, \phi_{\text{in}}] = 0 \tag{113}$$

for *all* operators ϕ_{in}. Therefore this operator must be a c-number (*i.e.,* proportional to the identity). Since $\lim_{t \to -\infty} H_{\text{int}}(\phi_{\text{in}}) = 0$ and $\lim_{t \to -\infty} U(t) = I$, this c-number must be equal to zero. We thus arrive to an operator equation for $U(t)$

$$i\partial_t U = H_{\text{int}}(\phi_{\text{in}}) \ U(t) \tag{114}$$

The operator U governs the time evolution of the states in the Interaction Representation, since the state $|\Phi\rangle_{\text{in}}$ becomes

$$U(t)|\Phi\rangle_{\text{in}} = |\Phi(t)\rangle \tag{115}$$

In particular, the *outgoing states* $|\Phi\rangle_{\text{out}}$ (*i.e.,* the states at $t \to +\infty$) are also *free states* which are related to the in-states by the operator $U(t)$ in the limit $t \to +\infty$

$$|\Phi\rangle_{\text{out}} = \lim_{t \to +\infty} U(t)|\Phi\rangle_{\text{in}} \equiv \hat{S}|\Phi\rangle_{\text{in}} \tag{116}$$

where $\hat{S} = \lim_{t \to +\infty} U(t)$ is the *S-matrix*.

23

The equation of motion for $U(t)$ can formally be solved using methods that we have discussed before. The solution is

$$U(t) = T e^{-i \int_{-\infty}^{t} dt' H_{\text{int}}(\phi_{\text{in}}(t'))} \tag{117}$$

where T is the time-ordering operator. In terms of the interaction part $\mathcal{L}_{\text{int}}$ of the Lagrangian we get

$$\hat{S} = \lim_{t \to +\infty} U(t) = T e^{-i \int_{-\infty}^{+\infty} dt' H_{\text{int}}(\phi_{\text{in}}(t'))} = T e^{i \int d^4x \, \mathcal{L}_{\text{int}}(\phi_{\text{in}})} \tag{118}$$

10.3.2 Physical Information Contained in the S-Matrix

Let us compute transition matrix elements between arbitrary *in* and *out* states. Let $|i, \text{in}\rangle$ be the initial incoming state and $|f, \text{out}\rangle$ the final outgoing state. The transition probability $W_{i \to f}$ is then given by

$$W_{i \to f} = |\langle f, \text{out}|i, \text{in}\rangle|^2 \equiv |\langle f, \text{in}|\hat{S}|i, \text{in}\rangle|^2 \tag{119}$$

since

$$\langle f, \text{out}|\hat{S} = \langle f, \text{in}| \tag{120}$$

We can split $\hat{S}$ into non-interacting and interacting parts

$$\hat{S} = \hat{I} + i\hat{T} \tag{121}$$

where $\hat{I}$ (the non-interacting part) is the identity operator, and $\hat{T}$, the T-matrix represents the interactions (not to be confused with the time-ordering symbol!). In terms of the T-matrix, the transition probability is

$$W_{i \to f} = |\langle f|i\rangle + i\langle f|T|i\rangle|^2 \tag{122}$$

Although from now on we will discuss the case of a scalar field, the arguments can be generalized to all other problems of interest with only minor modifications.

Let us consider the situation in which the initial state $|i, \text{in}\rangle$ consists of two wave packets which only contain positive frequency components

$$|i, \text{in}\rangle = \int \frac{d^3p}{2p_1^0(2\pi)^3} \int \frac{d^3p_2}{2p_2^0(2\pi)^3} f_1(p_1) f_2(p_2) |p_1, p_2; \text{in}\rangle \tag{123}$$

The incoming flux is equal to $\int \frac{d^3p}{2p_0(2\pi)^3} |f(p)|^2$. Each component $|p_1, p_2; \text{in}\rangle$ will have a matrix element with the final state $|f; \text{out}\rangle$. Since we have translation invariance, the total 4-momentum should be conserved. If we denote by P_f the momentum of the state $|f, \text{out}\rangle$, we can write

$$\langle f|T|p_1 p_2\rangle = (2\pi)^4 \delta^4(P_f - p_1 - p_2)\langle f|\mathcal{T}|p_1 p_2\rangle \tag{124}$$

24

where $\mathcal{T}$ is called the reduced operator. $\mathcal{T}$ acts only on the energy shell, $p^2 = m^2$. If we neglect the forward scattering contribution, the transition probability $W_{i \to f}$ becomes

$$
\begin{aligned}
W_{i \to f} \;=\; & \int \frac{d^3 p_1}{2 p_1^0 (2\pi)^3} \int \frac{d^3 p_2}{2 p_2^0 (2\pi)^3} \int \frac{d^3 q_1}{2 q_1^0 (2\pi)^3} \int \frac{d^3 q_2}{2 q_2^0 (2\pi)^3} \\
& (2\pi)^4 \delta^4(p_1 + p_2 - q_1 - q_2)\, (2\pi)^4 \delta^4(P_f - p_1 - p_2) \\
& f_1^*(p_1) f_2^*(p_2) f_1(q_1) f_2(q_2) \langle f | \mathcal{T} | p_1 p_2 \rangle^* \langle f | \mathcal{T} | q_1 q_2 \rangle
\end{aligned}
$$

(125)

The incoming states are assumed to be sharply peaked around some momenta $\bar{p}_1, \bar{p}_2$, with a spread Δp, such that we can approximate

$$
\langle f | \mathcal{T} | p_1 p_2 \rangle \approx \langle f | \mathcal{T} | q_1 q_2 \rangle \approx \langle f | \mathcal{T} | \bar{p}_1 \bar{p}_2 \rangle
$$

(126)

Under these assumptions, the form for the transition probability is

$$
W_{i \to f} = \int d^4 x |\widetilde{f}_1(x)|^2 |\widetilde{f}_2(x)|^2 (2\pi)^4 \delta^4(P_f - \bar{p}_1 - \bar{p}_2)|\langle f | \mathcal{T} | \bar{p}_1 \bar{p}_2 \rangle|^2
$$

(127)

where $\widetilde{f}(x)$ is the Fourier transform of $f(p)$. The integrand of Eq.(127) is the transition probability per unit time and volume

$$
\frac{dW_{i \to f}}{dt dV} = |\widetilde{f}_1(x)|^2 |\widetilde{f}(x)|^2 (2\pi)^4 \delta^4(P_f - \bar{p}_1 - \bar{p}_2)|\langle f | \mathcal{T} | \bar{p}_1 \bar{p}_2 \rangle|^2
$$

(128)

In position space, the flux is $i \int d^3 x \widetilde{f}^*(x) \overset{\leftrightarrow}{\partial_0} \widetilde{f}(x)$. If $\widetilde{f}(x)$ is sufficiently smooth, we can approximate

$$
i \widetilde{f}^*(x) \overset{\leftrightarrow}{\partial_0} \widetilde{f}(x) \approx 2 \bar{p}_0 |\widetilde{f}(x)|^2
$$

(129)

Let us assume that particle 1 is incident in the laboratory and that particle 2 is at rest in the lab. The density of particles in the target is

$$
\frac{dn_2}{dV} = 2 \bar{p}_2^0 |\widetilde{f}_2(x)|^2
$$

(130)

where $\bar{p}_2^0 = m_2$ since particle 2 is at rest. The incident flux is the velocity times the density of particles in the beam. Hence the incident flux Φ_{in} is

$$
\Phi_{\text{in}} = \frac{|\bar{p}_1|}{|\bar{p}_0^1|} 2 \bar{p}_1^0 |\widetilde{f}_1(x)|^2 = 2|\bar{p}_1| |\widetilde{f}_1(x)|^2
$$

(131)

The *differential cross section $d\sigma$* is related to the transition probability by the relation

$$
\frac{dW_{i \to f}}{dt dV} = \frac{dn_2}{dV} \cdot \Phi_{\text{in}} \cdot d\sigma
$$

(132)

Hence

$$
\begin{aligned}
2 m_2 |\widetilde{f}_2(x)|^2 2 |\bar{p}_1| |\widetilde{f}_1(x)|^2 d\sigma = \\
|\widetilde{f}_1(x)|^2 |\widetilde{f}_2(x)|^2 (2\pi)^4 \delta^4(P_f - \bar{p}_1 - \bar{p}_2)|\langle f | \mathcal{T} | \bar{p}_1 \bar{p}_2 \rangle|^2
\end{aligned}
$$

(133)

25

Therefore, the differential cross section $d\sigma$ is

$$d\sigma = (2\pi)^4 \delta^4(P_f - \bar{p}_1 - \bar{p}_2) \frac{1}{4 m_2 |\bar{p}_1|} |\langle f| \mathcal{T} |\bar{p}_1 \bar{p}_2 \rangle|^2 \qquad (134)$$

The quantity in the denominator $m_2 |\bar{p}_1|$ can be written in the relativistic invariant way

$$m_2 |\bar{p}| = m_2 \sqrt{\bar{p}_1^{02} - m_1^2} = \left[(\bar{p}_2 \cdot \bar{p}_1)^2 - m_1^2 m_2^2 \right]^{1/2} \qquad (135)$$

Thus far we have not made any assumptions about the nature of the final state. If the process that we consider involve two particles going into n particles. the

2 incoming
particles

n outgoing
particles
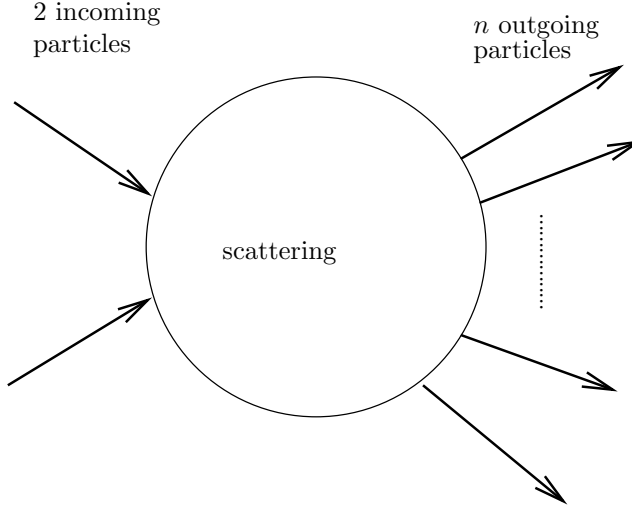
scattering

Figure 14: A $2 \to n$ scattering process.

total differential cross-section becomes

$$
\begin{aligned}
d\sigma \; = \; & \frac{1}{4 \left[(\bar{p}_2 \cdot \bar{p}_1)^2 - m_1^2 m_2^2 \right]^{1/2}} \int_\Delta \frac{d^3 p_3}{(2\pi)^3 2 p_3^0} \cdots \int_\Delta \frac{d^3 p_{n+2}}{(2\pi)^3 2 p_{n+2}^0} \\
& \times |\langle p_3, \ldots, p_{n+2} | \mathcal{T} | p_1 p_2 \rangle|^2 (2\pi)^4 \delta(p_1 + p_2 - \sum_{i=3}^{n+2} p_0)
\end{aligned}
$$
$$(136)$$

where Δ is an energy-momentum resolution. This expression shows that the central issue is to compute matrix elements of $\mathcal{T}$.

10.4 *Asymptotic States and the Analytic Properties of the Propagator*

We will show now that the S-matrix elements can be calculated if we know the v.e.v. of time-ordered products of field operators $\phi(x)$ in the Heisenberg representation. This is the LSZ (Lehmann, Symanzik and Zimmermann) approach.

In order to make this connection, it is necessary to relate the interacting fields $\phi(x)$ with a set of fields which create (or destroy) the actual states in the spectrum of the system, when these particles are far from each other. In any scattering experiment, the initial states are sharply peaked wave packets which can be constructed to be arbitrarily close to the eigenstates of the system. Of course, the true eigenstates are plane waves and any two such states will have a non-zero overlap in space. But wave packets which are essentially made of just one state will not overlap if the wave packets (the "particles") are far apart from each other at the initial time. Since they do not overlap, they do not interact. In this sense the spectrum of incoming states can be generated by a set of free fields. We will make the further assumption that the *in* and *out* states, the so-called *asymptotic states*, are created by a set of free fields. We will denote them by $\phi_{\text{in}}(x)$, and have the same form as the fields that appear in the Lagrangian. If the operators create the *actual* eigenstates, $\phi_{\text{in}}(x)$ must be a free field.

These assumptions amount to say that the states of the *fully interacting theory* are in *one-to-one correspondence* with the states of the non-interacting theory. In some loose sense, this hypothesis implies that the information that we can obtain from perturbation theory is qualitatively correct.

However, these assumptions can fail in several possible ways. A mild failure would be the appearance of *bound states* which, of course, are not present in the unperturbed theory. This situation is actually rather common and it can be remedied without too much difficulty. An example of this case is the Landau theory of the Fermi liquid and its collective modes. There are however at least two ways in which this picture can fail in a rather serious way. One case is the situation in which the fields of the Lagrangian do not describe any of the asymptotic states of the theory. An example of this case is Quantum Chromodynamics (QCD) whose Lagrangian describes the dynamics of *quarks* and *gluons* which are not present in the asymptotic states: *quarks* are *confined* and *gluons* are *screened*. The asymptotic states of QCD are mesons, baryons, and glue-balls which are *bound states* of quarks and gluons.

Another possible failure of this hypothesis is the case in which the states created by the fields of the Lagrangian are not the true elementary excitations but rather they behave like some effective composite object of some more elementary states. In such case the true one-particle states may be *orthogonal* to the states created by the fields of the Lagrangian. This is a rather common situation in theories in $1 + 1$ dimensions whose spectrum is generated by a set of soliton-like states, which are extended objects in terms of the bare fields of the Lagrangian. Something very similar happens in the theory of the fractional quantum Hall states.

In what follows, we will not consider these very interesting situations and

assume instead that these hypotheses (or scenarios) actually hold. For the sake of concreteness, we will deal with scalar fields, and we will require ϕ_{in} to satisfy the free Klein-Gordon equation

$$\left(\partial^2 + m^2\right)\phi_{\text{in}} = 0 \tag{137}$$

where m is the *physical mass*. In general, the physical mass is different from the mass parameter m_0 which enters in the Lagrangian of the interacting theory. As time goes by, this initial state evolves and the particles approach each other and begin to overlap. Interactions take place and, after some time, the system evolves to some final state which consists of a set of well defined particles, the out state. The unitary operator that connects in and out states is precisely the S-matrix of the interaction representation. The only difference here, resides in the fact that the in and out states *are not* eigenstates of some unperturbed system, but the actual eigenstates of the full theory.

This picture assumes that there is a stable vacuum state $|0\rangle$ such that the observed particles are the elementary excitations of this vacuum. The free fields $\phi_{\text{in}}(x)$ are just a device to generate the spectrum and have no real connection with actual dynamics. On the other hand, the interacting field $\phi(x)$ creates not only one-particle states but also many particle states. This is so because its equations of motion are non-linear. Hence the matrix element of $\phi(x)$ and $\phi_{\text{in}}(x)$ between the vacuum $|0\rangle$ and in-one-particle states $|1\rangle$, are generally different since ϕ_{in} creates *only* one-particle states. This must be true even as $t \to -\infty$. We state this difference by writing

$$\langle 1|\phi(x)|0\rangle = Z^{1/2}\langle 1|\phi_{\text{in}}|0\rangle \tag{138}$$

The proportionality constant Z is known as the wave-function renormalization. If $Z \neq 1$, the operator $\phi(x)$ must have a non-zero multi-particle projection. Notice that this is an identity of these matrix elements only. It is not an identity between the fields themselves.

In the interaction representation it is possible to derive a similar looking identity which originates from the fact that the unperturbed and perturbed states do not have the same normalization. It is important to stress that this approach makes the *essential* assumption that the states that are reached through perturbation theory in the interaction representation can approximate with arbitrary precision *all* of the *exact* states of the theory. This assumption is the hypothesis that the asymptotic states are generated by free fields.

The physical asymptotic states satisfy canonical commutation relations and the commutator of a pair of much fields is

$$\langle 0|[\phi_{\text{in}}(x), \phi_{\text{in}}(x')]|0\rangle = i\Delta(x - x'; m) \tag{139}$$

where m is the physical mass. On the other hand, the interacting fields satisfy

$$\langle 0|[\phi(x), \phi(x')]|0\rangle = \sum_n \left[\langle 0|\phi(x)|n\rangle\langle n|\phi(x')|0\rangle - (x \leftrightarrow x')\right] \tag{140}$$

28

where $\{|n\rangle\}$ is a complete set of physical (in) states. The operators $\phi(x)$ are related to the operator $\phi(0)$ (*i.e.*, at the origin at some time $x_0 = 0$) by

$$\phi(x) = e^{iP \cdot x} \phi(0) e^{-iP \cdot x} \tag{141}$$

where P_μ is the *total* 4-momentum operator. If we let P_n^μ be the 4-momentum of the state $|n\rangle$, we can write

$$\langle 0|[\phi(x), \phi(x')]|0\rangle = \sum_n \left[\langle 0|\phi(0)|n\rangle e^{-iP_n \cdot (x-x')} \langle n|\phi(0)|0\rangle - (x \leftrightarrow x') \right] \tag{142}$$

We now insert the identity

$$1 = \int d^4Q \, \delta^4(Q - P_n) \tag{143}$$

to get

$$\langle 0|[\phi(x), \phi(x')]|0\rangle = \int d^4Q \, \sum_n \delta^4(Q - P_n)|\langle 0|\phi(0)|n\rangle|^2 \left(e^{-iQ \cdot (x-x')} - e^{iQ \cdot (x-x')} \right) \tag{144}$$

We can summarize this result in terms of a *spectral density* $\rho(Q)$

$$\langle 0|[\phi(x), \phi(x')]|0\rangle = \int \frac{d^4Q}{(2\pi)^3} \rho(Q) \left(e^{-iQ \cdot (x-x')} - e^{iQ \cdot (x-x')} \right) \tag{145}$$

where $\rho(Q)$ given by

$$\rho(Q) = (2\pi)^3 \sum_n \delta^4(Q - P_n)|\langle 0|\phi(0)|n\rangle|^2 \tag{146}$$

Let us recall that $\Delta(x - x'; m)$ is given by

$$\begin{aligned}
i\Delta(x - x'; m) &= \int \frac{d^3Q}{(2\pi)^3 2Q_0} \left(e^{-iQ \cdot (x-x')} - e^{iQ \cdot (x-x')} \right) \\
&= \int \frac{d^4Q}{(2\pi)^3} \epsilon(Q^0) \delta^4(Q^2 - m^2) e^{-iQ \cdot (x-x')}
\end{aligned} \tag{147}$$

where $\epsilon(Q^0) = \text{sign}(Q^0)$. Thus we can write

$$\langle 0|[\phi(x), \phi(x')]|0\rangle = \int \frac{d^4Q}{(2\pi)^3} \rho(Q) \epsilon(Q^0) e^{-iQ \cdot (x-x')} \tag{148}$$

Since $\rho(Q)$ is Lorentz invariant by construction, it can only be a positive function of Q^2

$$\rho(Q) = \sigma(Q^2) > 0 \tag{149}$$

Hence

$$\langle 0|[\phi(x), \phi(x')]|0\rangle = \int \frac{d^4Q}{(2\pi)^3} \sigma(Q^2) \epsilon(Q^0) e^{-iQ \cdot (x-x')} \tag{150}$$

29

We will now rewrite this expression in the form of an integral over the spectrum. Let us insert the identity

$$1 = \int_0^\infty d\mu^2 \delta(Q^2 - \mu^2) \tag{151}$$

to obtain

$$\begin{aligned}
\langle 0|[\phi(x), \phi(x')]|0\rangle &= \int \frac{d^4Q}{(2\pi)^3} \left[\int_0^\infty d\mu^2 \delta(Q^2 - m'^2)\right] \sigma(Q^2)\epsilon(Q_0)e^{-iQ\cdot(x-x')} \\
&= \int_0^\infty d\mu^2 \sigma(\mu^2) \left[\int \frac{d^4Q}{(2\pi)^3} \epsilon(Q_0)\delta(Q^2 - \mu^2)e^{-iQ\cdot(x-x')}\right]
\end{aligned} \tag{152}$$

where $\sigma(\mu^2)$ is

$$\sigma(\mu^2) = (2\pi)^3 \sum_n \delta(P_n^2 - \mu^2)|\langle 0|\phi(0)|n\rangle|^2 \tag{153}$$

Thus, we can write the v. e. v. of the commutator as

$$\langle 0|[\phi(x), \phi(x')]|0\rangle = i \int_0^\infty d\mu^2 \sigma(\mu^2)\Delta(x - x'; m'^2) \tag{154}$$

If we assume that the theory has a *physical particle* with mass m (*i.e.,* one-particle states of mass m) we can write the final expression

$$-i\langle 0|[\phi(x), \phi(x')|0\rangle = Z\Delta(x - x'; m^2) + \int_{m_1^2}^\infty d\mu^2 \sigma(\mu^2)\Delta(x - x'; \mu^2) \tag{155}$$

where the first term represents the one-particle states and the integral represents the continuum of multi-particle states with a threshold at m_1. In other words, if there is a stable particle with mass m, the spectral function must have a δ-function at $m'^2 = m^2$ with strength Z, the spectral weight of the one-particle state.

Since the field $\phi(x)$ obeys equal-time canonical commutation relations with the momentum $\Pi(x) = \partial_0\phi(x)$, we get

$$\begin{aligned}
-i\langle 0|[\Pi(\vec{x}, x_0), \phi(\vec{x}', x_0)]|0\rangle = {} & Z \lim_{x_0' \to x_0} \partial_0\Delta(x - x'; m^2) \\
& + \int_{m_1^2}^\infty d\mu^2 \sigma(\mu^2) \lim_{x_0' \to x_0} \partial_0\Delta(x - x'; \mu^2)
\end{aligned} \tag{156}$$

On the other hand, the free field commutator $\Delta(x - x'; m^2)$ obeys the initial condition

$$\lim_{x_0' \to x_0} \partial_0\Delta(x - x'; m^2) = \lim_{x_0' \to x_0} [\Pi(x), \phi(x')] = -i\delta^3(\vec{x} - \vec{x}') \tag{157}$$

Hence, we find that the spectral function obeys the following identity (known as the *spectral sum rule*)

$$1 = Z + \int_{m_1^2}^{\infty} d\mu^2 \sigma(\mu^2) \tag{158}$$

From the positivity of $\sigma(m'^2)$ we get, $0 \leq Z \leq 1$. The lower end of the integration range, the threshold for multi-particle production m_1^2 is equal to $4m^2$ since, at least, we must create two elementary excitations. A similar analysis can be
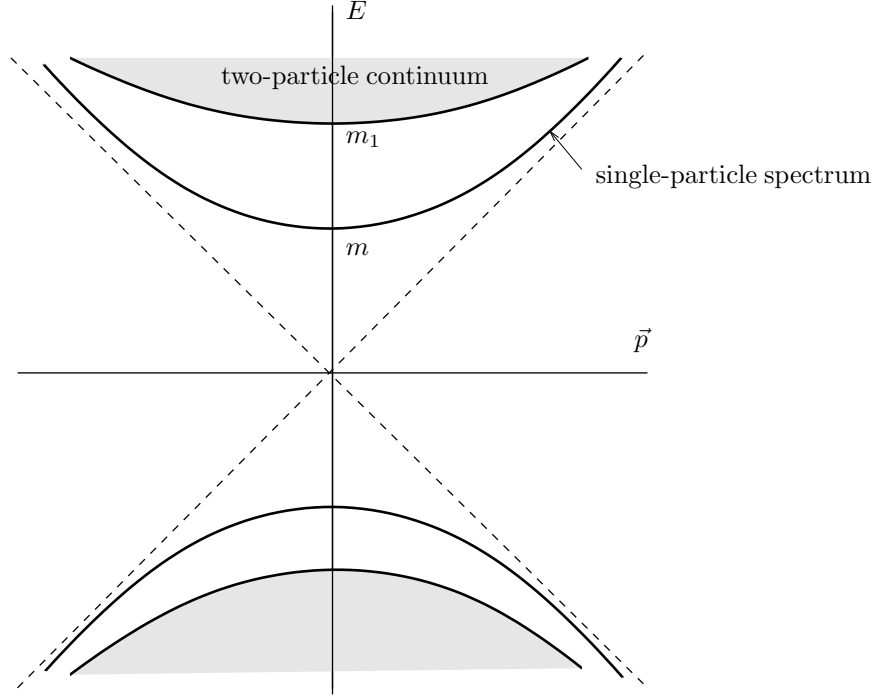
Figure 15: Spectrum of the propagator.

done for the Feynman (time-ordered) propagator

$$G_F(x - x'; m) = -i\langle 0|T\phi(x)\phi(x')|0\rangle \tag{159}$$

which has the *spectral representation*

$$G_F(x - x'; m) = Z G_0(x - x'; m) + \int_{m_1^2}^{\infty} d\mu^2 \sigma(\mu^2) G_0(x - x'; \mu^2) \tag{160}$$

This decomposition is known as the *Lehmann representation*. Here $G_0(x - x'; m^2)$ is the Feynman propagator for a free field

$$G_0(x - x') = -\int \frac{d^4 p}{(2\pi)^4} \frac{e^{-ip \cdot (x - x')}}{p^2 - m^2 + i\epsilon} \tag{161}$$

31

In the limit $\epsilon \to 0^+$, the poles of the integrand can be manipulated to give

$$\lim_{\epsilon \to 0^+} \frac{1}{p^2 - m^2 + i\epsilon} = \mathcal{P}\frac{1}{p^2 - m^2} - i\pi\delta(p^2 - m^2) \tag{162}$$

Using this identity we get that, in momentum space, the propagator is given by

$$G_F(p; m) = -\frac{Z}{p^2 - m^2 + i\epsilon} - \int_{m_1}^{\infty} d\mu^2 \frac{\sigma(\mu^2)}{p^2 - \mu^2 + i\epsilon} \tag{163}$$

Its imaginary part is given by

$$\text{Im } G_F(p; m) = \pi Z \, \delta(p^2 - m^2) + \pi \int_{m_1^2}^{\infty} \sigma(\mu^2)\delta(p^2 - \mu^2) \tag{164}$$

Hence

$$\frac{1}{\pi}\text{Im } G_F(p; m) = Z \, \delta(p^2 - m^2) + \sigma(p^2)\Theta(p^2 - m_1^2) \tag{165}$$
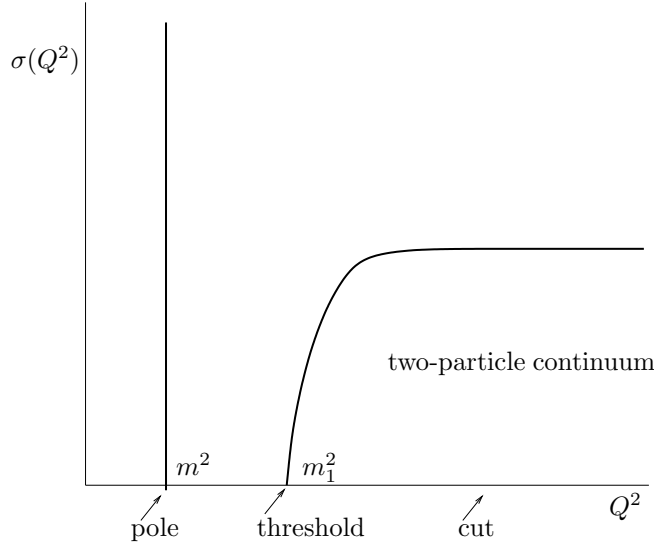
Figure 16: The analytic structure of the propagator is encoded in the spectral density $\sigma(Q^2)$.

Once the imaginary part is known, the real part is found through the *Kramers - Krönig* or *dispersion relation.*

$$\text{Re } G_F(p, m^2) = \frac{1}{\pi} \, \mathcal{P} \int_0^{\infty} d\mu^2 \, \frac{\text{Im } G_F(p, \mu^2)}{\mu^2 - p^2 - i\epsilon} \tag{166}$$

We see that, in general, there are two contributions to Im $G_F(p; m)$. The first term is the contribution from the single particle states. In addition, then

is a smooth contribution (the second term) which results form multi-particle production. While the single-particle states contribute with *an isolated pole* (a *δ-function* in the imaginary part), the multiple particle states (or continuum) are represented by a *branch cut*.

There is a simple and natural physical interpretation of these results. If the incoming state has $Q^2 < m^2$ it cannot propagate since the allowed value is at least, m^2 (the physical mass). If $Q^2 > m_1^2$, and if there are no bound states, the incoming state can *decay* into *at least* two single particle states. Hence $m_1^2 = 4m^2$. These states should form a continuum since given the initial momentum P_i there are many multi-particle states with the same total momentum. Thus, those processes are incoherent. Notice that without interactions, the incoming state would not have been able to decay into several single particle states.

We should stress that the propagators of all the theories that we have discussed have the same type of analytic structure that we have discussed here.

10.5 *The S-matrix and the Vacuum Expectation Value of Time Ordered Products of Fields*

We are now in position to find the connection between S-matrix elements and v. e. v. of time-ordered fields. For simplicity we will keep in mind the case of scalar fields but the results are easily generalizable. The actual derivation is rather lengthy and unilluminating. We will discuss its meaning and refer to standard texts for details.

Let's assume that we want to evaluate the matrix element

$$\langle p_1, \ldots, p_n; \text{out}|q_1, \ldots, q_m; \text{in}\rangle = \langle p_1, \ldots, p_n|\hat{S}|q_1, \ldots, q_m\rangle \qquad (167)$$

We will assume that all incoming and outgoing momenta are different. This matrix element is given by the *reduction formula*

$$\langle p_1, \ldots, p_n|\hat{S}|q_1, \ldots, q_m\rangle \quad = \quad \frac{i}{Z^{(n+m)/2}} \int d^4y_1 \ldots d^4y_n d^4x_1 \ldots d^4x_n$$

$$\times \exp\left[i(\sum_{\ell=1}^{n} p_\ell \cdot y_\ell - \sum_{k=1}^{m} q_k \cdot x_k)\right] \quad \prod_{\ell=1}^{n} \left(\partial_{y_\ell}^2 + m^2\right) \prod_{k=1}^{m} \left(\partial_{x_k}^2 + m^2\right)$$

$$\times \langle 0|T\left(\phi(y_1)\ldots\phi(y_n)\phi(x_1)\ldots\phi(x_m)\right)|0\rangle \qquad (168)$$

where m^2 is the physical mass and the external momenta p and q are on the mass shell, $p^2 = q^2 = m^2$.

Let us consider for example the $2 \to 2$ process

$$\langle p_1, p_2; \text{out}|q_1, q_2; \text{in}\rangle \quad = \quad \langle p_1 p_2, \text{in}|\hat{S}|q_1, q_2; \text{in}\rangle$$
$$= \quad \langle p_1 p_2, \text{out}|a_{\text{in}}^\dagger(q_1)|q_2, \text{in}\rangle$$

$$(169)$$

where $a_{\text{in}}^\dagger(q_1)$ is

$$
\begin{aligned}
a_{\text{in}}^\dagger(q_1) \;=\;& -i \int_{\text{fixed }t} d^3x \; \overset{\leftrightarrow}{\partial_0}\phi_{\text{in}}(x) \; e^{-iq_1 \cdot x} = \\
& \int d^3x \; (\omega(q)\phi_{\text{in}}(x) + i\Pi_{\text{in}}(x)) \; e^{-iq_1 \cdot x}
\end{aligned}
\tag{170}
$$

Hence, the matrix element is

$$
\begin{aligned}
\langle p_1 p_2 \text{out}|q_1 q_2 \text{in}\rangle \;=\;& -i \lim_{t \to -\infty} \int_t d^3x \; \overset{\leftrightarrow}{\partial_0}\langle p_1 p_2 \text{out}|\phi_{\text{in}}(x)|q_2 \text{in}\rangle \; e^{-iq_1 \cdot x} \\
\equiv\;& -i \lim_{t \to -\infty} \frac{1}{Z^{1/2}} \int_t d^3x \; \overset{\leftrightarrow}{\partial_0}\langle p_1 p_2 \text{out}|\phi(x)|q_2 \text{in}\rangle \; e^{-iq_1 \cdot x}
\end{aligned}
\tag{171}
$$

where we have made the replacement of ϕ_{in} by $\frac{1}{Z^{1/2}}\phi$ *inside* the matrix element $(t \to -\infty)$.

But

$$
\langle 0|\phi(x)|1\rangle = Z^{1/2}\langle 0|\phi_{\text{in}}(x)|1\rangle = Z^{1/2}\langle 0|\phi_{\text{out}}(x)|1\rangle
\tag{172}
$$

and

$$
\left(\lim_{t_f \to +\infty} - \lim_{t_i \to -\infty}\right)\int d^3x \; F(\vec{x}, t) = \lim_{t_f \to +\infty}\lim_{t_i \to -\infty}\int_{t_i}^{t_f} dt \; \frac{\partial}{\partial t}\int d^3x \; F(\vec{x}, t)
\tag{173}
$$

These formulas allow us to write

$$
\begin{aligned}
&\lim_{t_f \to +\infty}\int d^3x \; \langle p_1 p_2, \text{out}|a_{\text{in}}^\dagger(q_1)|q_2, \text{in}\rangle = \\
&= \lim_{t_i \to -\infty}\int d^3x \; \langle p_1 p_2, \text{out}|a_{\text{in}}^\dagger(q_1)|q_2, \text{in}\rangle + \int d^4x \; \partial_0 \langle p_1 p_2, \text{out}|a_{\text{in}}^\dagger(q_1)|q_2, \text{in}\rangle \\
&= \langle p_1 p_2, \text{out}|a_{\text{out}}^\dagger(q_1)|q_2, \text{in}\rangle
\end{aligned}
\tag{174}
$$

Thus, the matrix element is

$$
\begin{aligned}
\langle p_1 p_2, \text{out}|q_1 q_2, \text{in}\rangle =\;& \langle p_1 p_2, \text{out}|a_{\text{out}}^\dagger(q_1)|q_2 \text{in}\rangle \\
&+ \frac{i}{Z^{1/2}}\int d^4x \; \partial_0 \left[e^{-iq_1 \cdot x}\overset{\leftrightarrow}{\partial_0}\langle p_1 p_2 \text{out}|\phi(x)|q_2 \text{in}\rangle\right]
\end{aligned}
\tag{175}
$$

The first contribution is a *disconnected term* and it is given by

$$
\begin{aligned}
&\langle p_1 p_2 \text{out}|a_{\text{out}}^\dagger(q_1)|q_2 \text{in}\rangle \\
&= (2\pi)^3 2p_1^0\delta^3(p_1 - q_1)\langle p_2 \text{out}|q_1 \text{in}\rangle + (2\pi)^3 2p_2^0\delta^3(p_2 - q_1)\langle p_1 \text{out}|q_1 \text{in}\rangle
\end{aligned}
\tag{176}
$$

Notice that, if q_1 is on the mass shell, $q_1^2 = m^2$, and $e^{-iq_1 x}$ is a solution of the Klein-Gordon equation

$$(\partial^2 + m^2)e^{iq_1 \cdot x} = 0 \qquad (q_1^2 = m^2) \qquad (177)$$

The second contribution to the matrix element can also be evaluated (for arbitrary states α and β)

$$\int d^4x \, \partial_0 \left[e^{-iq_1 \cdot x} \overleftrightarrow{\partial_0} \langle \beta, \text{out}|\phi(x)|\alpha, \text{in}\rangle \right]$$

$$= \int d^4x \left[e^{-iq_1 \cdot x} \partial_0^2 \langle \beta, \text{out}|\phi(x)|\alpha, \text{in}\rangle + (-\partial_0^2 e^{-iq_1 \cdot x}) \langle \beta, \text{out}|\phi(x)|\alpha, \text{in}\rangle \right]$$

$$= \int d^4x \left[e^{-iq_1 \cdot x} \partial_0^2 \langle \beta, \text{out}|\phi(x)|\alpha, \text{in}\rangle + \left[\left(- \nabla^2 + m^2 \right) e^{-iq_1 \cdot x} \right] \langle \beta, \text{out}|\phi(x)|\alpha, \text{in}\rangle \right]$$

$$= \int d^4x e^{-iq_1 \cdot x} (\partial^2 + m^2) \langle \beta, \text{out}|\phi(x)|\alpha, \text{in}\rangle$$

$$(178)$$

where we have integrated by parts. Hence, the matrix element is

$$\langle p_1 p_2, \text{out}|q_1 q_2, \text{in}\rangle = \frac{i}{Z^{1/2}} \int d^4x_1 e^{-iq_1 \cdot x_1} (\partial^2 + m^2)\langle p_1 p_2, \text{out}|\phi(x_1)|q_2, \text{in}\rangle$$

$$+ (2\pi)^3 2p_1^0 \delta^3(p_1 - q_1) \quad \langle p_2, \text{out}|q_2, \text{in}\rangle + (2\pi)^3 2p_2^0 \delta^3(p_2 - q_1)\langle p_1, \text{out}|q_2, \text{in}\rangle$$

$$(179)$$

The matrix element inside the integrand of the first term is equal to

$$\langle p_1 p_2, \text{out}|\phi(x_1)|q_2, \text{in}\rangle = \lim_{y_1^0 \to +\infty} \frac{i}{Z^{1/2}} \int d^3 y_1 e^{ip_1 \cdot y_1} \overleftrightarrow{\partial_{y_1^0}} \langle p_2 \text{out}|\phi(y_1)|q_2 \text{in}\rangle$$

$$(180)$$

where (by definition) $y_1^0 > x_1^0$. This expression is also equal to

$$\langle p_1 p_2 \text{out}|\phi(x_1)|q_2 \text{in}\rangle = \langle p_2, \text{out}|\phi(x_1)a_{\text{in}}(p_1)|q_2, \text{in}\rangle$$

$$+ \frac{i}{Z^{1/2}} \int d^4 y_1 e^{ip_1 \cdot y_1} (\partial_{y_1}^2 + m^2)\langle p_2 \text{out}|T\phi(y_1)\phi(x_1)|q_2 \text{in}\rangle$$

$$(181)$$

By substituting back into the expression from the matrix element we find that the latter is equal to

$$\langle p_1 p_2, \text{out}|q_1 q_2, \text{in}\rangle =$$
$$(2\pi)^3 2p_1^0 \delta^3(p_1 - q_1)\langle p_2 \text{out}|q_2 \text{in}\rangle + (2\pi)^3 2p_2^0 \delta^3(p_2 - q_1)\langle p_1 \text{out}|q_2 \text{in}\rangle$$

$$+ \frac{i}{Z^{1/2}} \int d^4 x_1 e^{-iq_1 \cdot x_1} (\partial_{x_1}^2 + m^2)\langle p_2 \text{out}|\phi(x_1|0, \text{in}\rangle (2\pi)^3 2q_2^0 \delta^3(q_2 - p_1)$$

$$+ \left(\frac{1}{Z^{1/2}} \right)^2 \int d^4 x_1 d^4 y_1 e^{i(p_1 \cdot y_1 - q_1 \cdot x_1)} (\partial_{x_1}^2 + m^2)(\partial_{y_1}^2 + m^2)$$
$$\times \langle p_2 \text{out}|T\phi(y_1)\phi(x_1)|q_2 \text{in}\rangle$$

$$(182)$$

35

By iterating this process once more we obtain the *reduction formula* plus disconnected terms. The reduction formula provides the connection between the on-shell S-matrix elements and v. e. v. of time ordered products. Notice that the reduction formula implies that the Green functions must have poles in the variables p_1^2 (where p_i is conjugate to x_i) and that the matrix element is the residue of this pole. We will see later on that this residue is the on-shell one particle irreducible vertex function.

The reduction formula shows that all scattering data can be understood in terms of an appropriate v. e. v. of a time ordered product of field operators. The problem that we are left to solve is the computation of these v. e. v. 's. We will use perturbation theory to find them.

10.6 *Linear Response Theory*

In addition to the problem of evaluating S-matrix elements, it is of interest to consider the *response* of a system to weak localized external perturbations. These responses will tell us much about the nature of both the ground state and of the low-lying states of the system. This method is of great importance for the study of systems in condensed matter physics.

Let H be the full Hamiltonian of a system. We will consider the coupling of the system to weak external sources. Let $\hat{A}(x, t)$ be a *local observable* such as the charge density, the current density or the local magnetic moment. Let us represent the coupling to the external source by an extra term $H_{\text{ext}}(t)$ in the Hamiltonian. The total Hamiltonian now is

$$H_T = H + H_{\text{ext}} \tag{183}$$

If the source is adiabatically switched on and off, then the Heisenberg representation for the isolated system becomes the interaction representation for the full system. Hence, exactly as in the interaction representation, all the observables obey the Heisenberg equations of motion of the system in the absence of the external source while the states will follow the external source in their evolution. Namely, let $|\text{gnd}\rangle$ be the *exact* ground state (or vacuum) of the system in the absence of any external sources. The external sources perturb this ground state and cause the v.e.v. of the local observable $\hat{A}(x, t)$ to change:

$$\langle \text{gnd}|\hat{A}(\vec{x}, t)|\text{gnd}\rangle \to \langle \text{gnd}|U^{-1}(t)\ \hat{A}(\vec{x}, t)\ U(t)|\text{gnd}\rangle \tag{184}$$

where the time evolution operator $U(t)$ is now given by

$$U(t) = T \exp\{-\frac{i}{\hbar} \int_{-\infty}^{t} dt' H_{\text{ext}}(t')\} \tag{185}$$

Linear Response Theory consists in evaluating the changes in the expectation values of the observables to *leading order* in the *external perturbation*. Thus, to leading order in the external sources, the *change* is

$$\delta\langle \text{gnd}|\hat{A}(\vec{x}, t)|\text{gnd}\rangle = \frac{i}{\hbar} \int_{-\infty}^{t} dt'\ \langle \text{gnd}|[H_{\text{ext}}(t'), \hat{A}(\vec{x}, t)]|\text{gnd}\rangle + \ldots \tag{186}$$

Quite generally, we will be interested in the case in which H_{ext} represents the local coupling of the system to an external source $f(\vec{x}, t)$ through the observable $\hat{A}(\vec{x}, t)$. Thus, we will choose the perturbation $H_{\text{ext}}(t)$ to have the form

$$H_{\text{ext}}(t) = \int d^3x \, f(\vec{x}, t) \, \hat{A}(\vec{x}, t) \tag{187}$$

The function $f(\vec{x}, t)$ is usually called the *force*. If the observable is normal ordered relative to the ground state of the isolated system, *i.e.,* $\langle \text{gnd}|\hat{A}(\vec{x}, t)|\text{gnd}\rangle = 0$, the change of its expectation value will be equal to the final value and it is given by

$$\delta\langle \text{gnd}|\hat{A}(\vec{x}, t)|\text{gnd}\rangle_f = \frac{i}{\hbar} \int_{-\infty}^{t} dt' \int d^3x' \, \langle \text{gnd}|\hat{A}(\vec{x}, t'), \hat{A}(\vec{x}, t)]|\text{gnd}\rangle \, f(\vec{x}', t')+\cdots \tag{188}$$

The main assumption of Linear Response theory is that the *response* is *proportional* to the *force*. The proportionality constant is interpreted as a *generalized susceptibility* χ.

$$\delta\langle \text{gnd}|\hat{A}(\vec{x}, t)|\text{gnd}\rangle = \chi \cdot f \equiv \int d^3x' \int_{-\infty}^{t} dt' \, \chi(x, x') \, f(x') + \ldots \tag{189}$$

where $\chi(x, x')$ is the susceptibility.

Let $D^R(x, x')$ represent the *retarded Green function* of the observable $\hat{A}(\vec{x}, t)$,

$$D^R(x, x') = -i\Theta(x_0 - x_0')\langle \text{gnd}|[\hat{A}(x), \hat{A}(x')]|\text{gnd}\rangle \tag{190}$$

We see that $\langle A(x)\rangle$ is determined by $D^R(x, x')$ since

$$\delta\langle \text{gnd}|A(x)|\text{gnd}\rangle = \frac{1}{\hbar} \int d^4x' D^R(x, x')f(x') + \ldots \tag{191}$$

Therefore, the responses and the susceptibilities are given by retarded Green functions, not by time-ordered ones. However, since the retarded and time-ordered Green functions are related by an analytic continuation, the knowledge of the latter gives the information about the former.

Let us Fourier transform the time-dependence of $\langle A(\vec{x}, t)\rangle$. The Fourier transform, $\langle A(\vec{x}, \omega)\rangle$, is given by the expression

$$\delta\langle \text{gnd}|A(\vec{x}, \omega)|\text{gnd}\rangle =$$
$$\int d^3x' \left\{ -\frac{i}{\hbar} \int_{-\infty}^{0} d\tau \langle \text{gnd}|[A(\vec{x}, t), A(\vec{x}', t + \tau)]|\text{gnd}\rangle \, e^{i\omega\tau} \right\} f(\vec{x}\,', \omega) \tag{192}$$

where $f(\vec{x}, \omega)$ is the Fourier transform of $f(\vec{x}, t)$. Thus, the Fourier transform of the generalized susceptibility, $\chi(\vec{x}, \vec{x}\,'; \omega)$ is given by

$$\chi(\vec{x}, \vec{x}\,'; \omega) = -\frac{i}{\hbar} \int_{-\infty}^{0} d\tau \, e^{i\omega\tau} \, \langle \text{gnd}|[A(\vec{x}, 0)A(\vec{x}\,', \tau)]|\text{gnd}\rangle \tag{193}$$

which is known as the *Kubo Formula*. Hence

$$\chi(\vec{x}, \vec{x}\,'; \omega) = \frac{1}{\hbar} \int_{-\infty}^{+\infty} d\tau \; e^{i\omega\tau} D^R(x, x') \qquad (194)$$

If we also Fourier transform the space dependence, we get

$$\langle A(\vec{p}, \omega) \rangle = \frac{1}{\hbar} D^R(\vec{p}, \omega) f(\vec{p}, \omega) \qquad (195)$$

and the generalized susceptibility $\chi(\vec{p}, \omega)$ now becomes

$$\chi(\vec{p}, \omega) = \frac{\langle A(\vec{p}, \omega) \rangle}{f(\vec{p}, \omega)} = \frac{1}{\hbar} D^R(\vec{p}, \omega) \qquad (196)$$

In practice we will compute the *time-ordered* Green Function $D(x, x')$. If we recall our discussion about the propagator, we expect $D(\vec{p}, \omega)$ to have poles on the real frequency axis. For $D(x, x')$ to be time ordered, all the poles with $\omega < 0$ should be moved (infinitesimally) upwards into the complex frequency upper half-plane while all poles with $\omega > 0$ should be moved downwards into lower half-plane. Thus $D(p, \omega)$ is not analytic on either half-plane. The retarded Green function $D_R(p, \omega)$ is (with our conventions for Fourier transform) analytic in the lower half-plane. Thus we can relate $D(p, \omega)$ to $D^R(p, \omega)$ by

$$\begin{aligned}
\mathrm{Re}D^R(p, \omega) &= \mathrm{Re}D(p, \omega) & &\equiv \hbar\mathrm{Re}\chi(p, \omega) \\
\mathrm{Im}D^R(p, \omega) &= \mathrm{Im}D(p, \omega)\mathrm{sign}\omega & &\equiv \hbar\mathrm{Im}\chi(p, \omega)
\end{aligned} \qquad (197)$$

The time-ordered Green function $D(p, \omega)$ (the propagator for the observable $\hat{A}(x, t)$) admits a spectral (or Lehmann) representation similar to that of the propagator for the relativistic scalar field, Eq.(160). Similarly, we can define the *spectral function* $A(p, \omega)$ of the observable to be $A(p, \omega) = \mathrm{Im}D^{\mathrm{ret}}(p, \omega)$.

These relations imply that the susceptibility $\chi(p, \omega)$ obeys the Kramers-Krönig (or dispersion) relation

$$\mathrm{Re}\chi(p, \omega) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} d\omega' \; \frac{\mathrm{Im}\chi(p, \omega')}{\omega' - \omega} \qquad (198)$$

Finally, let us recast the formulas for a general change of an arbitrary operator into a more compact form. We can apply the formulas that we derived for the interaction representation just to the part of the Hamiltonian which involves the coupling to the external sources $H_{\mathrm{ext}}(t)$. The interaction representation S-matrix is

$$\hat{S} = \lim_{t \to +\infty} U(t) = T \; e^{-\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt H_{\mathrm{ext}}(t)} \qquad (199)$$

Let $\langle \mathrm{gnd}, \mathrm{out} | \mathrm{gnd}, \mathrm{in} \rangle$ be the *vacuum persistence amplitude*

$$\langle \mathrm{gnd}, \mathrm{out} | \mathrm{gnd}, \mathrm{in} \rangle = \langle \mathrm{gnd} | \hat{S} | \mathrm{gnd} \rangle = \langle \mathrm{gnd} | T \; e^{-\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \; H_{\mathrm{ext}}(t)} | \mathrm{gnd} \rangle \qquad (200)$$

which we denote by $Z[f]$

$$Z[f] = \langle \text{gnd}|T\, e^{-\frac{i}{\hbar}\int d^4x\, f(x)\, A(x)}|\text{gnd}\rangle \qquad (201)$$

By expanding in powers of $f(x)$ we get

$$\begin{aligned}Z[f] &= 1 - \frac{i}{\hbar}\int d^4x f(x)\langle \text{gnd}|A(x)|\text{gnd}\rangle \\ &+ \frac{1}{2!}(-\frac{i}{\hbar})^2 \int d^4x \int d^4x' f(x)f(x')\langle \text{gnd}|T\, A(x)A(x')|\text{gnd}\rangle + \ldots\end{aligned} \qquad (202)$$

The second term vanishes if $A(x,t)$ is normal ordered. Within the same degree of precision, we can re-exponentiate this expression to give

$$Z[f] = e^{\frac{i}{2\hbar}\int d^4x \int d^4x' f(x)K(x,x')f(x') + 0(f^3)} \qquad (203)$$

where the kernel $K(x,x')$ is the time-ordered Green function

$$K(x,x') = \frac{i}{\hbar}\langle \text{gnd}|T A(x)A(x')|\text{gnd}\rangle \qquad (204)$$

In general the observables of physical interest are, at least, bilinears in the fields. Thus, the kernels $K(x,x')$ represent not one-particle propagators but generally propagators for two or more excitations. We can learn a lot from a physical system if the spectral functions of the kernels $K(x,x')$ are known. In general we expect that the spectral function will have a structure similar to that of the propagator: one (or more) δ-function contributions and a branch cut. The δ-functions are two (or more) particle bound states known as collective modes. The branch cuts originate from the two or multi-particle continuum. Examples of collective modes are plasmons (sound waves) in electron liquids and spin waves in magnets.

10.6.1 Application of the Kubo Formula: Electrical Conductivity of a Metal

We will only consider the response of an electron gas to weak external electromagnetic fields $A_\mu(x)$. The formalism can be generalized easily to other systems and responses. In particular, we will consider the electrical conductivity of a metal.

There are three effects (and couplings) that we need to take into consideration: a) electrostatic, b) diamagnetic (or orbital) and c) paramagnetic. The electrostatic coupling is simply the coupling to an external potential with H_{ext} given by

$$H_{\text{ext}} = \sum_{\sigma=\uparrow,\downarrow} \int d^3x\, e\phi(x,t)\, \psi_\sigma^\dagger(x)\psi_\sigma(x) \qquad (205)$$

where $\phi \equiv A_0$ is the scalar potential (or time component of the vector potential A_μ). The diamagnetic coupling (or orbital) follows from the minimal coupling to the external vector potential $\vec{A}$. The kinetic energy term H_K is modified following the minimal coupling prescription to become

$$H_K(A) = \int d^3x \sum_{\sigma=\uparrow,\downarrow} \frac{\hbar^2}{2m} \left(\vec{\nabla} + \frac{ie}{\hbar c}\vec{A}(x) \right) \psi_\sigma^\dagger(x) \cdot \left(\vec{\nabla} - \frac{ie}{\hbar c}\vec{A}(\vec{x}) \right) \psi_\sigma(x) \quad (206)$$

which can be written as a sum of two terms

$$H_K(A) = H_K(0) + H_{\text{ext}}(A) \quad (207)$$

where $H_K(0)$ is the Hamiltonian in the absence of the field and $H_{\text{ext}}(A)$ is the perturbation, $i.e.,$

$$H_{\text{ext}}(A) = \int d^3x \left[\vec{J}(\vec{x}) \cdot \vec{A}(\vec{x}) - \frac{e^2}{2mc^2}\vec{A}^2(\vec{x}) \sum_\sigma \psi_\sigma^\dagger(\vec{x})\psi_\sigma(\vec{x}) \right] \quad (208)$$

Here $\vec{J}(\vec{x})$ is the gauge-invariant charge current

$$\begin{aligned}
\vec{J}(\vec{x}) &= \frac{ie\hbar}{2mc} \sum_\sigma \left[\psi_\sigma^\dagger(\vec{x})\vec{\nabla}\psi_\sigma(\vec{x}) - \vec{\nabla}\psi^\dagger(\vec{x})\psi(\vec{x}) \right] - \frac{e^2}{mc^2}\vec{A}(\vec{x}) \sum_\sigma \psi_\sigma^\dagger(\vec{x})\psi_\sigma(\vec{x}) \\
&\equiv \frac{ie\hbar}{2mc} \sum_\sigma \left[\psi_\sigma^\dagger(\vec{x})\vec{D}\psi_\sigma(\vec{x}) - \left(\vec{D}\psi_\sigma(\vec{x}) \right)^\dagger \psi_\sigma(\vec{x}) \right]
\end{aligned}$$
$$(209)$$

Clearly $\vec{J}(\vec{x})$ is the sum of the two terms, one which represents the mass current and the diamagnetic term, $\frac{e^2}{mc^2}\vec{A}^2 \sum_\sigma \psi_\sigma^\dagger\psi_\sigma$. We can write the total perturbation, including the scalar potential A_0, if we write

$$H_{\text{ext}} = \int d^3x \left[J_\mu(x)A^\mu(x) - \frac{e^2}{2mc^2}\vec{A}^2 \sum_\sigma \psi_\sigma^\dagger\psi_\sigma \right] \quad (210)$$

Finally, we can also consider a paramagnetic coupling to the spin degrees of freedom which has the Zeeman form

$$H_{\text{ext}}^{\text{Zeeman}} = \int d^3x\, g\vec{B}(\vec{x}) \cdot \sum_{\sigma,\sigma'} \psi_\sigma^\dagger(\vec{x})\vec{S}_{\sigma\sigma'}\psi_{\sigma'}(\vec{x}) \quad (211)$$

where g is typically of the order of the Bohr magneton μ_B and $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$ for spin one-half systems.

A straightforward application of the Linear Response formulas derived above yields an expression for the current $\langle J_\mu \rangle'$ in the presence of the perturbation.

$$\langle J_\mu(x) \rangle' = \langle J_\mu(x) \rangle_{\text{gnd}} - \frac{i}{\hbar} \int_{-\infty}^t dt' \int d^3x' \langle \text{gnd}|[J_\nu(x'), J_\mu(x)]|\text{gnd}\rangle A_\nu(x') \quad (212)$$

This formula suggests that we should define the *retarded current correlation function* $\mathcal{D}_{\mu\nu}^R(x, x')$

$$\mathcal{D}_{\mu\nu}^{\text{Ret}}(x, x') = -i\Theta(x_0 - x_0')\langle\text{gnd}|[J_\mu(x), J_\nu(x')]|\text{gnd}\rangle \tag{213}$$

The *induced current* $\langle J_\mu\rangle_{\text{ind}}$

$$\langle J_\mu\rangle_{\text{ind}} = \langle J_\mu\rangle' - \langle j_\mu\rangle_{\text{gnd}} \tag{214}$$

(where j_μ is the mass current) has a very simple form in terms of $\mathcal{D}_{\mu\nu}^R(x, x')$, namely

$$\langle J_\mu(x)\rangle_{\text{ind}} = \frac{1}{\hbar}\int d^4x' \mathcal{D}_{\mu\nu}^{\text{Ret}}(x, x')A^\nu(x') - \frac{e^2}{mc^2}A_k(x)\langle n(x)\rangle\delta_{\mu k} + O(A^2) \tag{215}$$

Below we will show that $\langle J_\mu(x)\rangle_{\text{ind}}$ is (a) conserved (*i.e.*, $\partial_\mu^x\langle J^\mu(x)\rangle_{\text{ind}} = 0$) and (b) gauge-invariant.

Since $\langle J_\mu(x)\rangle_{\text{ind}}$ is gauge invariant, we can compute its form in any gauge. In the gauge $A_0 = 0$ the spatial components of $\langle J_\mu(x)\rangle_{\text{ind}}$ are

$$\langle J_k(x)\rangle_{\text{ind}} = -\frac{e^2\rho}{mc^2}A_k(x) + \int d^4x' \mathcal{D}_{k\ell}^{\text{ret}}(x - x')A_\ell(x') + O(A^2) \tag{216}$$

In this gauge, the external electric field $\vec{E}_{\text{ext}}$ and magnetic field $\vec{H}$ are

$$\vec{E}_{\text{ext}} = -\partial_0\vec{A} \qquad \vec{H} = \vec{\nabla}\times\vec{A} \tag{217}$$

Now, in Fourier space, we can write

$$\begin{aligned}
\langle J_k(\vec{p}, \omega)\rangle_{\text{ind}} &= -\frac{e^2\rho}{mc^2}A_k(\vec{p}, \omega) + \mathcal{D}_{k\ell}^{\text{ret}}(\vec{p}, \omega)A_\ell(\vec{p}, \omega) \\
&\equiv \left(\mathcal{D}_{k\ell}^{\text{ret}}(\vec{p}, \omega) - \frac{e^2\rho}{mc^2}\delta_{k\ell}\right)\frac{E_\ell^{\text{ext}}}{i\omega}(p, \omega)
\end{aligned} \tag{218}$$

This expression is *almost* the conductivity. It is not quite that since the conductivity is a relation between the *total current* $\vec{J} = \vec{J}_{\text{ind}} + \vec{J}_{\text{ext}}$ and the *total electric field* $\vec{E}$. In order to take these electromagnetic effects into account, we must use Maxwell's equations in a medium, which involve $\vec{E}, \vec{D}, \vec{B}$ and $\vec{H}$

$$\begin{aligned}
\vec{\nabla}\cdot\vec{D} = \rho \qquad \vec{\nabla}\times\vec{E} = -\frac{\partial\vec{H}}{\partial t} \\
\vec{\nabla}\cdot\vec{B} = 0 \qquad \vec{\nabla}\times\vec{H} = \frac{\partial\vec{E}}{\partial t} + \vec{J}
\end{aligned} \tag{219}$$

where

$$\vec{B} = \vec{H} + \vec{M} \qquad \vec{E} = \vec{E}^{\text{ext}} + \vec{E}^{\text{ind}} \tag{220}$$

Here $\vec{M}$ and $\vec{E}^{\text{ind}}$ are the magnetic and electric polarization vectors. In particular

$$\vec{J}^{\text{ind}} = \partial_t\vec{E}^{\text{ind}} \tag{221}$$

and
$$\partial_t \vec{D} = \partial_t \vec{E} + \vec{J}^{\text{ind}} \tag{222}$$

Linear Response theory is the statement that $\vec{D}$ must be proportional to $\vec{E}$,
$$D_j = \varepsilon_{jk} E_k \tag{223}$$

where ε_{jk} is the dielectric tensor. Since $\vec{E}$ and $\vec{E}^{\text{ext}}$ satisfy similar equations

$$
\begin{aligned}
-\vec{\nabla} \times \vec{\nabla} \times \vec{E} &= \partial_t^2 \vec{E} + \partial_t \vec{J} \\
-\vec{\nabla} \times \vec{\nabla} \times \vec{E}^{\text{ext}} &= \partial_t^2 \vec{E}^{\text{ext}} + \partial_t \vec{J}^{\text{ext}}
\end{aligned}
\tag{224}
$$

Since $\vec{\nabla} \times \vec{\nabla} \times \vec{E} = \vec{\nabla}(\vec{\nabla} \cdot \vec{E}) - \nabla^2 \vec{E}$, we can write, for the Fourier transforms, the equations

$$
\begin{aligned}
p_i p_j E_j(\vec{p}, \omega) - \vec{p}^2 E_i(\vec{p}, \omega) &= -\omega^2 E_j(\vec{p}, \omega) - i\omega J_i(\vec{p}, \omega) \\
p_i p_j E_j^{\text{ext}}(\vec{p}, \omega) - \vec{p}^2 E_i^{\text{ext}}(\vec{p}, \omega) &= -\omega^2 E_i^{\text{ext}}(\vec{p}, \omega) - i\omega J_i^{\text{ext}}(\vec{p}, \omega)
\end{aligned}
\tag{225}
$$

Thus, we get

$$
\begin{aligned}
p_i p_j E_j(\vec{p}, \omega) - \vec{p}^2 E_i(\vec{p}, \omega) \quad + \quad & \omega^2 E_i(\vec{p}, \omega) = -i\omega J_i^{\text{ind}}(\vec{p}, \omega) \\
+ \quad & p_i p_j E_j^{\text{ext}}(\vec{p}, \omega) - \vec{p}^2 E_i^{\text{ext}}(\vec{p}, \omega) + \omega^2 E_i^{\text{ext}}(\vec{p}, \omega)
\end{aligned}
\tag{226}
$$

and
$$-i\omega J_i^{\text{ind}}(\vec{p}, \omega) = \left(\delta_{ij} \frac{e^2 \rho}{mc^2} - \mathcal{D}_{ij}^R(\vec{p}, \omega) \right) E_j^{\text{ext}}(\vec{p}, \omega) \tag{227}$$

from where we conclude that

$$
\begin{aligned}
(p_i p_j - \vec{p}^2 \delta_{ij} \quad + \quad & \omega^2 \delta_{ij}) E_j(\vec{p}, \omega) = \\
& (\delta_{ij} \frac{e^2 \rho}{mc^2} - \mathcal{D}_{ij}^R(\vec{p}, \omega) + p_i p_j - \vec{p}^2 \delta_{ij} + \omega^2 \delta_{ij}) E_j^{\text{ext}}(\vec{p}, \omega)
\end{aligned}
\tag{228}
$$

In matrix form, these equations have the simpler form

$$(p \otimes p - \vec{p}^2 I + \omega^2 I)\vec{E} = \left(\frac{e^2 \rho}{mc^2} I - \mathcal{D}^R + p \otimes p - \vec{p}^2 I + \omega^2 I \right) \vec{E}_{\text{ext}} \tag{229}$$

This equation allows us to write $\vec{E}_{\text{ext}}$ in terms of $\vec{E}$. We find that the induced current is

$$
\begin{aligned}
i\omega \vec{J}_{\text{ind}} = & \\
& \left(\mathcal{D}^R - \frac{e^2 \rho}{mc^2} I \right) \left[\frac{e^2 \rho}{mc^2} I - \mathcal{D}^R + p \otimes p - \vec{p}^2 I + \omega^2 I \right]^{-1} \left(p \otimes p - \vec{p}^2 I + \omega^2 I \right) \vec{E}
\end{aligned}
\tag{230}
$$

and we find that the *conductivity tensor* σ is

$$i\omega\sigma(\vec{p},\omega) = \left(\mathcal{D}^R(\vec{p},\omega) - \frac{e^2\rho}{mc^2}I\right) +$$

$$\left(\mathcal{D}^R(\vec{p},\omega) - \frac{e^2\rho}{mc^2}I\right)\left[\frac{e^2\rho}{mc^2}I - \mathcal{D}^R(\vec{p},\omega) + p\otimes p - \vec{p}^2I + \omega^2I\right]^{-1}\left(\mathcal{D}^R(\vec{p},\omega) - \frac{e^2\rho}{mc^2}I\right)$$

$$(231)$$

Also, since $\vec{D} = \varepsilon\vec{E}$, the dielectric tensor ε is

$$\varepsilon = I + \frac{i}{\omega}\,\sigma \tag{232}$$

10.6.2   Correlation Functions and Conservation Laws

In the problem discussed in the previous section, we saw that we had to consider a correlation function of currents. Since the currents are conserved, *i.e.,*

$$\partial_\mu J^\mu = 0, \tag{233}$$

we expect that the correlation function $\mathcal{D}_{\mu\nu}(x,x')$ should obey a similar equation. Let us compute the divergence of the retarded correlation function,

$$\partial_\mu^x \mathcal{D}_{\text{ret}}^{\mu\nu}(x,x') = \partial_\mu^x\left(-i\Theta(x_0 - x_0')\langle\text{gnd}|[J^\mu(x), J^\nu(x')]|\text{gnd}\rangle\right) \tag{234}$$

Except for the contribution coming from the step function, we see that we can operate with the derivative inside the expectation value to get

$$\begin{aligned}\partial_\mu^x \mathcal{D}_{\text{ret}}^{\mu\nu}(x,x') &= -i\left(\partial_\mu^x\Theta(x_0 - x_0')\right)\langle\text{gnd}|[J^\mu(x), J^\nu(x')]|\text{gnd}\rangle \\ &\quad -i\Theta(x_0 - x_0')\langle\text{gnd}|[\partial_\mu^x J^\mu(x), J^\nu(x')]|\text{gnd}\rangle\end{aligned}$$

$$(235)$$

The second term vanishes since $J^\mu(x)$ is a conserved current and the first term is non zero only if $\mu = 0$. Hence we find

$$\partial_\mu^x \mathcal{D}_{\text{ret}}^{\mu\nu}(x,x') = -i\delta(x_0 - x_0')\langle\text{gnd}|\left[J^0(x), J^\nu(x')\right]|\text{gnd}\rangle \tag{236}$$

which is the v.e.v. of an equal-time commutator. These commutators are given by

$$\begin{aligned}\langle\text{gnd}|\left[J^0(\vec{x}, x_0), J^0(\vec{x}, x_0)\right]|\text{gnd}\rangle &= 0 \\ \langle\text{gnd}|\left[J^0(\vec{x}, x_0), J^i(\vec{x}', x_0)\right]|\text{gnd}\rangle &= \frac{ie^2}{mc^2}\partial_k^x\left[\delta(\vec{x} - \vec{x}')\langle n(\vec{x})\rangle\right]\end{aligned}$$

$$(237)$$

Hence, the divergence of $\mathcal{D}_{\mu\nu}^{\text{ret}}$ is

$$\partial_x^\mu \mathcal{D}_{\mu k}^{\text{ret}}(x,x') = \frac{e^2}{mc^2}\partial_k^x\left[\delta^4(x - x')\langle n(x)\rangle\right] \quad ; \quad \partial_{x'}^\mu \mathcal{D}_{0\mu}^{\text{ret}}(x,x') = 0 \tag{238}$$

and

$$\partial_{x'}^{\nu} \mathcal{D}_{k\nu}^{\text{ret}}(x, x') = -\frac{e^2}{mc^2} \partial_k^x \left[\delta^4(x - x') \langle n(x') \rangle \right] \quad ; \quad \partial_{x'}^{\mu} \mathcal{D}_{0\mu}^{\text{ret}}(x, x') = 0 \quad (239)$$

Notice that the time-ordered functions also satisfy these identities. These identities can be used to prove that $\langle \vec{J}^{\text{ind}} \rangle$ is indeed gauge-invariant and conserved. Furthermore, in momentum and frequency space, the identities become

$$
\begin{aligned}
-i\omega \mathcal{D}_{00}^R(\vec{p}, \omega) - ip_k \mathcal{D}_{k0}^R(\vec{p}, \omega) &= 0 \\
-i\omega \mathcal{D}_{0k}^R(\vec{p}, \omega) - ip_\ell \mathcal{D}_{\ell k}^R(\vec{p}, \omega) &= -\frac{e^2 \bar{n}}{mc^2} ip_k \\
-i\omega \mathcal{D}_{00}^R(p, \omega) - ip_k \mathcal{D}_{0k}^R(\vec{p}, \omega) &= 0 \\
-i\omega \mathcal{D}_{k0}^R(\vec{p}, \omega) - ip_\ell \mathcal{D}_{k\ell}^R(\vec{p}, \omega) &= -\frac{e^2 \bar{n}}{mc^2} ip_k
\end{aligned}
$$

$$(240)$$

We can combine these identities to get

$$\omega^2 \mathcal{D}_{00}^R(\vec{p}, \omega) - p_\ell p_k \mathcal{D}_{\ell k}^R(\vec{p}, \omega) = -\frac{e^2 \bar{n}}{mc^2} \vec{p}^{\,2} \qquad (241)$$

Hence, the density-density and the current-current correlation functions are not independent. A number of interesting identities follow from this equation. In particular if we take the static limit $\omega \to 0$ at fixed momentum $\vec{p}$, we get

$$\lim_{\omega \to 0} p_\ell p_k \mathcal{D}_{\ell k}^{\text{ret}}(\vec{p}, \omega) = \frac{e^2 \bar{n}}{mc^2} \vec{p}^{\,2} \qquad (242)$$

provided that $\lim_{\omega \to 0} \mathcal{D}_{00}^{\text{ret}}(\vec{p}, \omega)$ is not singular for $\vec{p} \neq 0$. Also from the equal-time commutator

$$\langle \text{gnd} | [J_k(\vec{x}, x_0), J_0(\vec{x}, x_0)] | \text{gnd} \rangle = \frac{ie^2}{mc^2} \partial_k^x \left(\delta(\vec{x} - \vec{x}') \langle n(x) \rangle \right) \qquad (243)$$

we get

$$\lim_{x_0' \to x_0} \partial_k^x \mathcal{D}_{k0}^{ret}(x, x') = \frac{e^2}{mc^2} \nabla_x^2 \left(\delta(x - x') \langle n(x) \rangle \right) \qquad (244)$$

If the system is uniform, $\langle n(x) \rangle = \bar{n} = \rho$, we can Fourier transform this identity to get

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} ip_k \mathcal{D}_{k0}^{\text{ret}}(\vec{p}, \omega) = -\frac{e^2 \bar{n}}{mc^2} \vec{p}^{\,2} \qquad (245)$$

The conservation laws yield the alternative expression

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} i\omega \mathcal{D}_{00}^{\text{ret}}(\vec{p}, \omega) = \frac{e^2 \bar{n}}{mc^2} \vec{p}^{\,2} \qquad (246)$$

which is known as the *f-sum rule*.

44

If the system is isotropic, these relations can be used to yield a simpler form for the conductivity tensor. Indeed, for an isotropic system $\mathcal{D}_{k\ell}^{\text{ret}}(\vec{p}, \omega)$ can only have the form of a sum of a longitudinal part $\mathcal{D}_{\parallel}^{\text{ret}}$ and a transverse part $\mathcal{D}_{\perp}^{\text{ret}}$

$$\mathcal{D}_{\ell k}^{\text{ret}}(\vec{p}, \omega) = \mathcal{D}_{\parallel}^{\text{ret}}(\vec{p}, \omega)\frac{p_\ell p_k}{\vec{p}^{\,2}} + \mathcal{D}_{\perp}^{\text{ret}}(\vec{p}, \omega)\left(\frac{p_\ell p_k}{\vec{p}^{\,2}} - \delta_{\ell k}\right) \tag{247}$$

Thus, we get a relation between $\mathcal{D}_{00}^{\text{ret}}$ and $\mathcal{D}_{\parallel}^{\text{ret}}$

$$\omega^2 \mathcal{D}_{00}^{\text{ret}}(p, \omega) - \vec{p}^{\,2}\mathcal{D}_{\parallel}^{\text{ret}}(\vec{p}, \omega) = -\frac{e^2 \bar{n}}{mc^2}\vec{p}^{\,2} \tag{248}$$

Hence

$$\mathcal{D}_{00}^{\text{ret}}(\vec{p}, \omega) = \frac{\vec{p}^{\,2}}{\omega^2}\left(\mathcal{D}_{\parallel}^{\text{ret}}(\vec{p}, \omega) - \frac{e^2 \bar{n}}{mc^2}\right) \tag{249}$$

and

$$\lim_{\omega \to 0} \mathcal{D}_{\parallel}^{\text{ret}}(\vec{p}, \omega) = \frac{e^2 \bar{n}}{mc^2} \tag{250}$$

for all $\vec{p}$.

The conductivity tensor can also be separated into longitudinal $\sigma_{\parallel}$ and transverse $\sigma_{\perp}$ pieces

$$\sigma_{ij} = \sigma_{\parallel}\frac{p_i p_j}{\vec{p}^{\,2}} + \sigma_{\perp}\left(\frac{p_i p_j}{\vec{p}^{\,2}} - \delta_{ij}\right) \tag{251}$$

we find

$$\sigma_{\parallel} = i\omega\left[\frac{\mathcal{D}_{\parallel}^{\text{ret}} - \frac{e^2 \bar{n}}{mc^2}}{-\mathcal{D}_{\parallel}^{\text{ret}} + \frac{e^2 \bar{n}}{mc^2} + \omega^2}\right] \tag{252}$$

and

$$\sigma_{\perp} = \frac{1}{i\omega}\left(\mathcal{D}_{\perp}^{\text{ret}} - \frac{e^2 \bar{n}}{mc^2}\right)\left[1 + \frac{\mathcal{D}_{\perp}^{\text{ret}} - \frac{e^2 \bar{n}}{mc^2}}{\frac{e^2 \bar{n}}{mc^2} - \mathcal{D}_{\perp}^{\text{ret}} + \omega^2 - \vec{p}^{\,2}}\right] \tag{253}$$

These relations tell us that the real part of $\sigma_{\parallel}$ is determined by the imaginary part of $\mathcal{D}_{\parallel}^{\text{ret}}$. Thus, the *resistive part* of $\sigma_{\parallel}$ (which is responsible for dissipation in the system) is determined by the imaginary part of a response function. This is generally the case.

A The Dirac Propagator in a Background Electromagnetic Field and Coulomb Scattering

Let us consider briefly the Dirac propagator in a background electromagnetic field and use it to compute the S-matrix for Coulomb scattering. By a background field we mean a classical (fixed but possibly time-dependent) electromagnetic field $A_\mu(x)$. We will denote by $S_F(x, x'|A)$ the Dirac propagator in a background field A_μ. $S_F(x, x'|A)$ obeys the Green function equation

$$\left(i\slashed{\partial} - e\slashed{A} - m\right)S_F(x, x'|A) = \delta^4(x - x') \tag{254}$$

whereas the Dirac propagator $S_F(x, x')$ in the absence of a background field obeys instead

$$\left(i\slashed{\partial} - m\right) S_F(x, x') = \delta^4(x - x') \tag{255}$$

Thus, we can also write Eq.(254) as

$$\left(S_F^{-1} - e\slashed{A}\right) S_F(A) = 1 \tag{256}$$

Hence

$$S_F(x, x'|A) = S_F(x - x') + e \int d^4y \, S_F(x - y) \, \slashed{A}(y) \, S_F(y, x'|A) \tag{257}$$

or, in components,

$$S_F^{\alpha\beta}(x, x'|A) = S_F^{\alpha\beta}(x - x') + e \int d^4y \, S_F^{\alpha\lambda}(x - y) \, [A_\mu(y)\gamma^\mu]^{\lambda\sigma} \, S_F^{\sigma\beta}(y, x'|A) \tag{258}$$

As an explicit application we will consider the case of Coulomb scattering of Dirac electrons from a fixed nucleus with positive electric charge Ze. We will now compute the S-matrix for this problem in the Born approximation. As in non-relativistic Quantum Mechanics, in this approximation we replace the propagator in the integrand of Eqs. (257) and (258) by the free Dirac propagator, $S_F(x - x')$.

Consider now an incoming state, a spinor the we will denote by $\Psi_i(x)$, with a particle with positive energy (an electron) and spin up (say in the z direction), and momentum $\vec{p}_i$. This incoming (initial) state is (for $x_0 \to -\infty$)

$$\Psi_i(x) = \frac{1}{\sqrt{V}} \, u^{(\alpha)}(p_i) \, \sqrt{\frac{m}{E_i}} \, e^{-ip_i \cdot x} \tag{259}$$

The outgoing (final) state $\Psi_f(x)$ is a spinor representing also a particle with positive energy (an electron) with spin up (also in the z direction) and momentum $\vec{p}_f$, and it is given by

$$\Psi_f(y) = \frac{1}{\sqrt{V}} \, u^{(\beta)}(p_f) \, \sqrt{\frac{m}{E_f}} \, e^{-ip_f \cdot y} \tag{260}$$

The S-matrix is

$$S_{fi} = i \lim_{x_0 \to -\infty} \lim_{y_0 \to +\infty} \int d^3x \int d^3y \, \overline{\Psi}_f(\vec{y}, y_0) \, S_F(y, x|A) \, \Psi_i(\vec{x}, x_0) \tag{261}$$

At the level of the Born approximation we can write

$$\begin{aligned}
S_{fi} = \; & i \lim_{x_0 \to -\infty} \lim_{y_0 \to +\infty} \int d^3x \int d^3y \, \overline{\Psi}_f(\vec{y}, y_0) \, S_F(y, x) \, \Psi_i(\vec{x}, x_0) + \\
& i \lim_{x_0 \to -\infty} \lim_{y_0 \to +\infty} \int d^3x \int d^3y \int d^4z \, \overline{\Psi}_f(\vec{y}, y_0) \, S_F(y, z) \, \slashed{A}(z) \, S_F(z, x) \, \Psi_i(\vec{x}, x_0) + \dots
\end{aligned} \tag{262}$$

We now recall the expression for the free Dirac propagator

$$S_F(x - x' = -i\langle 0|T\psi_\alpha(x)\bar\psi_{\alpha'}(x')|0\rangle$$
$$= -i\int \frac{d^3p}{(2\pi)^3} \left(\frac{m}{E(p)}\right) \left(\theta(x_0' - x_0)e^{-ip \cdot (x' - x)}\Lambda_+(p) + \theta(x_0 - x_0')e^{-ip \cdot (x - x'}\Lambda_-(p)\right)$$

$$(263)$$

where $\Lambda_\pm(p)$ are projection operators onto positive (particle) and negative (anti-particle) energy states:

$$\Lambda_\pm(p) = \frac{1}{2m}\left(\pm\slashed{p} + m\right) \tag{264}$$

Alternatively, we can express the propagator in terms of the basis spinors $u^\sigma(p)$ (which span the positive energy states), and $v^\sigma(p)$ (which span the negative energy states), as

$$S_F(x' - x) = -i\theta(x_0' - x_0)\int d^3p \sum_{\sigma=1,2} u_p^{(\sigma)}(x')\bar u_p^{(\sigma)}(x)$$
$$+i\theta(x_0 - x_0')\int d^3p \sum_{\sigma=1,2} v_p^{(\sigma)}(x')\bar v_p^{(\sigma)}(x)$$

$$(265)$$

where we have used the notation

$$u_p^{(\sigma)}(x) \equiv u^{(\sigma)}(p)\, e^{-ip \cdot x}, \quad v_p^{(\sigma)}(x) = v^{(\sigma)}(p)\, e^{-ip \cdot x} \tag{266}$$

Let us begin by computing first the top line in Eq.(262), the projection of the free propagator onto the initial and final states. By expanding the propagator we find,

$$\int d^3x d^3y\, \bar\psi_f(y)S_F(y - x)\psi_i(x) =$$
$$-i\theta(y_0 - x_0)\int d^3p \sum_{\sigma=1,2}\int d^3x d^3y\, \bar\psi_f(y)u_p^{(\sigma)}(y)\bar u_p^{(\sigma)}(x)\psi_i(x)$$
$$+i\theta(x_0 - y_0)\int d^3p \sum_{\sigma=1,2}\int d^3x d^3y\, \bar\psi_f(y)v_p^{(\sigma)}(y)\bar v_p^{(\sigma)}(x)\psi_i(x)$$

$$(267)$$

We now use the orthogonality relations of the Dirac basis spinors to find

$$\int d^3y\, \bar\psi_f^{(\beta)}(y)u_p^{(\sigma)}(y) = \delta^{\beta\sigma}\delta^3(\vec p - \vec p_f)$$
$$\int d^3x\, \bar u_p^{(\sigma)}(x)\psi_i^{(\alpha)}(x) = \delta^{\sigma\alpha}\delta^3(\vec p - \vec p_i)$$

$$(268)$$

Hence, to leading order the matrix element S_{fi} of the S-matrix is

$$S_{fi} = \delta^3(\vec{p}_f - \vec{p}_i)\delta^{\alpha\beta} + \text{Born term} \tag{269}$$

Let us now compute the Born term (the first Born approximation). We will need to compute first an expression for

$$\int d^3y \; \bar{\psi}_f(y) S_F(y, z) \tag{270}$$

and for

$$\int d^3x \; S_F(z, x)\psi_i(x) \tag{271}$$

Using once again the expansion of the propagator we find that Eq.(270) is

$$\int d^3y \; \bar{\psi}_f(y) S_F(y, z) =$$

$$\int d^3y \; \bar{\psi}_f^{(\beta)}(y)(-i)\theta(y_0 - z_0) \sum_{\sigma=1,2} \int d^3p \; u_p^{(\sigma)}(y)\bar{u}_p^{(\sigma)}(z)$$

$$+ \int d^3y \; \bar{\psi}_f^{(\beta)}(i)\theta(z_0 - y_0) \sum_{\sigma=1,2} v_p^{(\sigma)}(y)\bar{v}_p^{(\sigma)}(z)$$

$$= -i\theta(y_0 - z_0) \sum_{\sigma=1,2} \int d^3p \left(\int d^3y \; \bar{\psi}_f^{(\beta)}(y)u_p^{\sigma)}(y) \right) \bar{u}_p^{(\sigma)}(z)$$

$$+i\theta(z_0 - y_0) \sum_{\sigma=1,2} \int d^3p \left(\int d^3y \; \bar{\psi}_f^{(\beta)}(y)v_p^{\sigma)}(y) \right) \bar{v}_p^{(\sigma)}(z)$$

$$= \begin{cases} -i\theta(y_0 - z_0) \; \bar{\psi}_f^{(\beta)}(z), & \text{if the final state is a particle} \\ +i\theta(z_0 - y_0) \; \bar{\psi}_f^{(\beta)}(z), & \text{if the final state is an antiparticle} \end{cases} \tag{272}$$

The other expression, Eq.(271), can be computed similarly. Putting it all together we find that the Born term is

$$\text{Born term} = -ie \int d^4z \; \bar{\psi}_f^{(\beta)}(z) \; A\!\!\!/ \psi_i^{(\alpha)}(z) \; \theta(y_0 - z_0) \; \theta(z_0 - x_0) \tag{273}$$

corresponding to an electron propagating forward in time.

Let us evaluate this expression for the case of a Coulomb potential,

$$A^\mu = (A_0, 0), \quad A_0 = \frac{-Ze}{4\pi r} \tag{274}$$

with $r = |\vec{z}|$. The Born term now becomes

$$\begin{aligned} \text{Born term} = \; &-ie \int_{-\infty}^{\infty} dz_0 \int d^3z \; \bar{\psi}_f^{(\beta)}(z)\gamma_0\psi_i^{(\alpha)}(z) \; \theta(y_0 - z_0) \left(\frac{-Ze}{4\pi r} \right) \\ = \; &\frac{ie}{V} \frac{m}{\sqrt{E_i E_f}} \frac{Ze}{4\pi} \int_{-\infty}^{\infty} dz_0 \int d^3z \; e^{i(p_f - p_i)\cdot z} \frac{1}{r} \; \bar{u}^{(\beta)}(p_f)\gamma_0 u^{(\alpha)}(p_i) \end{aligned} \tag{275}$$

48

where V is the volume. Using now that

$$\int_{-\infty}^{\infty} dz_0 \, e^{i(E_f - E_i)z_0} = 2\pi\delta(E_f - E_i) \qquad (276)$$

we can write the Born term as

$$\text{Born term} = \frac{iZ\alpha}{V} \frac{m}{\sqrt{E_iE_f}} \frac{1}{2\pi\delta(E_i - E_f)} \int d^3r \, \frac{e^{-i\vec{q}\cdot r}}{r} \, \bar{u}^{(\beta)}(p_f)\gamma_0 u^{(\alpha)}(p_i) \qquad (277)$$

where $\alpha = \frac{e^2}{4\pi}$ is the fine structure constant, $\vec{q} = \vec{p}_f - \vec{p}_i$ is the momentum transfer, and

$$\int d^3r \, \frac{e^{-i\vec{q}\cdot r}}{r} = \frac{4\pi}{|\vec{q}|} \qquad (278)$$

The matrix element of the S-matrix, in the Born approximation, is then equal to

$$S_{fi} = \delta^{\alpha\beta}\delta^3(\vec{p}_f - \vec{p}_i) + i\frac{Z\alpha}{V} \frac{M}{\sqrt{E_iE_f}} \, 2\pi\delta(E_i - E_f) \frac{4\pi}{q^2} \, \bar{u}^{(\beta)}(p_f)\gamma_0 u^{(\alpha)}(p_i) \qquad (279)$$

Since

$$\text{\# states with } \vec{p}_f \text{ within } d^3p_f = V\frac{d^3p_f}{(2\pi)^3} \qquad (280)$$

we can write the transition probability per particle into these final states as

$$|S_{fi}|^2 \, V \frac{d^3p_f}{(2\pi^3)} = Z^2 \frac{(4\pi\alpha)^2}{E_iV} \, m^2 \, \frac{|\bar{u}^{(\beta)}(p_f)\gamma_0 u^{(\alpha)}(p_i)|^2}{|\vec{q}|^4} \, \frac{d^3p_f}{(2\pi)^3 E_f} \, 2\pi\delta(E_f - E_i) \, T \qquad (281)$$

where T is the time of measurement (this is Fermi's Golden rule).

Thus, the number of transitions per particle and unit time is

$$\frac{dP_{fi}}{dt} = \int |\frac{iZ\alpha}{V} \frac{m}{\sqrt{E_fE_i}} \frac{4\pi}{|\vec{q}|^2} \, \bar{u}^{(\beta)}(p_f)\gamma_0 u^{(\alpha)}(p_i)|^2 \, 2\pi\delta(E_f - E_i)V\frac{d^3p_f}{(2\pi)^3} \qquad (282)$$

Dividing out this expression by the incoming flux, $\frac{1}{V}\frac{|\vec{p}_i|}{E_i}$, we obtain an expression for the differential cross section

$$d\sigma_{fi} = \left(\int dp_f p_f^2 \, \frac{4Z^2\alpha^2 m^2}{|\vec{p}_i|E_f|\vec{q}|^4} |\bar{u}^{(\beta)}(p_f)\gamma_0 u^{(\alpha)}(p_i)|^2\delta(E_f - E_i)\right)^2 d\Omega_f \qquad (283)$$

For elastic scattering, $|\vec{p}_i| = |\vec{p}_f| = p_f$ and $EdE = p_fdp_f$, we obtain that the differential cross section is

$$d\sigma_{fi} = \frac{4Z^2\alpha^2 m^2}{|\vec{q}|^4}|\bar{u}^{(\beta)}(p_f)\gamma_0 u^{(\alpha)}(p_i)|^2 d\Omega_f \qquad (284)$$

For an unpolarized beam we get

$$\left.\frac{d\sigma_{fi}}{d\Omega}\right|_{\text{unpolarized}} = \frac{Z^2\alpha^2}{4|\vec{p}|^2\beta^2\sin^4(\theta/2)}\left(1 - \beta^2\sin^2\frac{\theta}{2}\right) \qquad (285)$$

where $\beta = v/c$.