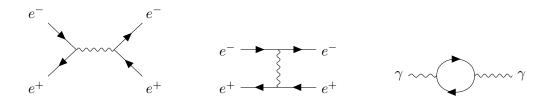
An Introduction to Quantum Field Theory - Part I

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"The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing abstraction." – Sidney Coleman

Quantum field theory is the most complete and consistent theoretical framework that provides a unified description of quantum mechanics and special relativity. In the limit $\hbar \to 0$ we obtain relativistic classical fields which can be used to describe for example electrodynamics. In the limit of small velocities $v/c \ll 1$, we obtain non-relativistic quantum mechanics. Finally in the limit $\hbar \to 0$ and $v/c \ll 1$ we obtain the description of non-relativistic classical fields such as sound waves.

Fields are described by a function which assigns a value to every point on the base manifold which we consider. In this course we will be mostly looking at relativistic quantum field theory, which is defined in 3+1 -dimensional Minkowski space-time. Most results can be straightforwardly translated to other systems, like 2-dimensional systems in condensed matter physics.

The notes are very brief and obviously only give an introduction to quantum field theory. The following books provide more detailed explanations and also more in-depth knowledge about quantum field theory.

- 1. M. Srednicki, "Quantum Field Theory"
- 2. M. Schwartz, "Quantum Field Theory and the Standard Model"
- 3. L. Ryder, "Quantum Field Theory"
- 4. M. Peskin, D. Schroeder, "An Introduction to Quantum Field Theory"
- 5. S. Weinberg, "The Quantum Theory of Fields", Vol. 1
- 6. C. Itzykson, J-B. Zuber, "Quantum Field Theory"
- 7. D. Bailin, "Introduction to Gauge Field Theory"
- 8. A. Zee, "Quantum Field Theory in a Nutshell"

The notes follow the same notation as Srednicki's book. In particular we will use natural units

$$\hbar = c = k_B = 1$$

and the signature (-+++) for the metric. Thus length scales and time are measured with the same units

$$[\ell] = [t] = \frac{1}{[m]} = \frac{1}{[E]} = \frac{1}{[T]} = eV^{-1}$$

which is the inverse of energy. Temperature is measure in the same units as energy.

Often we will use formal manipulations which require a more mathematical treatment. In quantum field theory we will encounter many divergences which have to be regulated. This is generally possible by considering a finite volume V and to quantize the theory in this finite volume. In the infinite volume limit we obtain $V \to (2\pi)^3 \delta^{(3)}(0)$ which is divergent. See arXiv:1201.2714 [math-ph] for some lecture notes with a more rigorous discussion of different mathematical issues in quantum field theory.

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1 Spin 0 – scalar field theory

1.1 Relativistic classical field theory

An intuitive derivation of the Klein-Gordon equation. Any theory of fundamental physics has to be consistent with relativity as well as quantum theory. In particular a particle with 4-momentum p^{μ} have to satisfy the relativistic dispersion relation

$$p^{\mu}p_{\mu} = -E^2 + \vec{p}^2 = -m^2 \ . \tag{1.1}$$

Following the standard practice in quantum mechanics we replace the energy and momentum by operators

$$E \to i\hbar \partial_t$$
 $\vec{p} \to -i\hbar \vec{\nabla}$ (1.2)

and postulate the wave equation for a relativistic spin-0 particle

$$-m^{2}\phi = -(i\partial_{t})^{2} + (-i\vec{\nabla})^{2}\phi = (\partial_{t}^{2} - \vec{\nabla}^{2})\phi \qquad (\Box - m^{2})\phi = 0$$
 (1.3)

which is the so-called Klein-Gordon equation. The Klein-Gordon equation is solved in terms of plane waves $\exp(i\vec{k}\cdot\vec{x}\pm i\omega_k t)$ with $\omega_k=(\vec{k}^2+m^2)^{1/2}$ and thus the general solution is given by their superposition

$$\phi(x,t) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left(a(k)e^{i\vec{k}\cdot\vec{x} - i\omega_k t} + b(k)e^{i\vec{k}\cdot\vec{x} + i\omega_k t} \right)$$
(1.4)

The factor $1/\omega_k$ ensures that the integral measure $\int d^3k/(2\pi)^3 2\omega_k$ is Lorentz invariant, i.e. invariant under orthochronous Lorentz transformations ($\Lambda_0^0 \ge 1$). This can be directly seen from noticing that ¹

$$\int_{-\infty}^{\infty} dk^0 \delta(k^2 + m^2) \theta(k^0) = \frac{1}{2\omega_k} , \qquad (1.6)$$

since there is only one zero at $k^0 = \omega_k$ for $k^0 > 0$. Thus we can rewrite the integration in terms of $d^4k\delta(k^2+m^2)\theta(k^0)$ with the Dirac δ -function and the Heaviside step function θ which is manifestly Lorentz invariant. For a real scalar field $[\phi(x,t) = \phi^*(x,t)]$, the coefficients a and b are related by $b(k) = a^*(-k)$. Thus for a real scalar field we find

$$\phi(x,t) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left(a(k)e^{ik_\mu x^\mu} + a^*(k)e^{-ik_\mu x^\mu} \right)$$
 (1.7)

where we changed the integration variable $\vec{k} \to -\vec{k}$ for the second term. If we were to interpret the solution as a quantum wave function, the second term would correspond to "negative energy" contributions.

$$\int dx \delta(f(x)) = \sum_{i} \frac{1}{|f'(x_i)|} \tag{1.5}$$

where x_i are zeros of the function f.

¹Note that

Using the representation of the δ function

$$(2\pi)^3 \delta^{(3)}(\vec{k}) = \int d^3x e^{i\vec{k}\cdot\vec{x}}$$
 (1.8)

we can invert Eq. (1.7) to obtain

$$\int d^3x e^{-ik_{\mu}x^{\mu}}\phi(x) = \frac{1}{2\omega_k}a(k) + \frac{1}{2\omega_k}e^{2i\omega_k t}a^*(-k)$$
 (1.9)

$$\int d^3x e^{-ik_{\mu}x^{\mu}} \partial_0 \phi(x) = -\frac{i}{2}a(k) + \frac{i}{2}e^{2i\omega_k t}a^*(-k)$$
(1.10)

and thus we obtain for the coefficients a(k)

$$a(k) = \int d^3x e^{-ik_{\mu}x^{\mu}} \left[\omega_k + i\partial_0\right] \phi(x) = i \int d^3x \ e^{-ik_{\mu}x^{\mu}} \stackrel{\leftrightarrow}{\partial_0} \phi(x) \ . \tag{1.11}$$

with $f(x) \stackrel{\leftrightarrow}{\partial_x} g(x) \equiv f(x) \partial_x g(x) - (\partial_x f(x)) g(x)$.

1.2 Stationary action principle

This equation can also be derived from the least action principle using the following Lagrangian density

$$\mathcal{L} = -\frac{1}{2}\partial_{\mu}\phi\partial^{\mu}\phi - \frac{1}{2}m^{2}\phi^{2} \tag{1.12}$$

and thus the action $S = \int dt \int d^3x \mathcal{L}$. Consider a variation of the action with respect to the field ϕ and the coordinates x^{μ}

$$x'^{\mu} = x^{\mu} + \delta x^{\mu} \qquad \qquad \phi'(x) = \phi(x) + \delta \phi(x) \qquad (1.13)$$

and thus the total variation of ϕ is $\Delta \phi = \delta \phi + (\partial_{\mu} \phi) \delta x^{\mu}$. Variation of the action yields

$$\delta S = \int_{R} d^{4}x' \mathcal{L}(\phi', \partial_{\mu}\phi', x') - \int_{R} d^{4}x \mathcal{L}(\phi, \partial_{\mu}\phi, x)$$
(1.14)

$$= \int_{R} d^{4}x \left(\frac{\partial \mathcal{L}}{\partial \phi} \delta \phi + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \delta(\partial_{\mu} \phi) + \frac{\partial \mathcal{L}}{\partial x^{\mu}} \delta x^{\mu} + \mathcal{L} \partial_{\mu} \delta x^{\mu} \right)$$
(1.15)

$$= \int_{R} d^{4}x \left(\frac{\partial \mathcal{L}}{\partial \phi} - \partial_{\mu} \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \right) \delta \phi + \int_{R} d^{4}x \partial_{\mu} \left(\mathcal{L} \delta x^{\mu} + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \delta \phi \right)$$
(1.16)

$$= \int_{R} d^{4}x \left(\frac{\partial \mathcal{L}}{\partial \phi} - \partial_{\mu} \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \right) \delta \phi + \int_{\partial R} d\sigma_{\mu} \left(\mathcal{L} \delta x^{\mu} + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \delta \phi \right)$$
(1.17)

where we used $\det(\frac{\partial x'^{\mu}}{\partial x^{\lambda}}) = \delta^{\mu}_{\lambda} + \partial_{\lambda} \delta x^{\mu}$ in the second line. If we demand on the boundary ∂R that there is no variation in the fields $\delta x^{\mu} = 0$ and $\delta \phi = 0$, we obtain the Euler-Lagrange equations

$$0 = \frac{\partial \mathcal{L}}{\partial \phi} - \partial_{\mu} \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \tag{1.18}$$

For a real scalar field the Euler-Lagrange equation is

$$0 = \frac{\delta \mathcal{L}}{\delta \phi} - \partial_{\mu} \frac{\delta \mathcal{L}}{\delta \partial_{\mu} \phi} = \partial_{\mu} \partial^{\mu} \phi - m^{2} \phi . \tag{1.19}$$

The conjugate momentum to the field ϕ is

$$\pi = \frac{\partial \mathcal{L}}{\partial \partial_0 \phi} \tag{1.20}$$

and the Hamiltonian density is obtained by a Legendre transformation

$$\mathcal{H} = \pi \dot{\phi} - \mathcal{L} \tag{1.21}$$

The Poisson brackets for two functionals $L_{1,2}$ are defined as²

$$\{L_1, L_2\}_{\phi,\pi} = \int d^3x \left[\frac{\delta L_1}{\delta \phi(x,t)} \frac{\delta L_2}{\delta \pi(x,t)} - \frac{\delta L_1}{\delta \pi(x,t)} \frac{\delta L_2}{\delta \phi(x,t)} \right] . \tag{1.24}$$

and thus the Poisson brackets for the field ϕ and conjugate momentum π are

$$\{\phi(x,t), \pi(y,t)\} = \delta^3(x-y) \tag{1.25}$$

$$\{\pi(x,t),\pi(y,t)\} = \{\phi(x,t),\phi(y,t)\} = 0 \tag{1.26}$$

and Hamilton's equation for $f = f(\phi, \pi)$ reads

$$\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t} \tag{1.27}$$

1.3 Symmetries and Noether's theorem

For an arbitrary surface ∂R we can rewrite the second integral as

$$\int_{\partial R} d\sigma_{\mu} \left(\mathcal{L} \delta x^{\mu} + \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \delta \phi \right) = \int_{\partial R} d\sigma_{\mu} \left[\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \Delta \phi - \Theta^{\mu}_{\nu} \delta x^{\nu} \right]$$
(1.28)

where we defined the energy-momentum tensor (see below)

$$\Theta^{\mu}_{\ \nu} \equiv \frac{\partial \mathcal{L}}{\partial(\partial_{\mu}\phi)} \partial_{\nu}\phi - \mathcal{L}\delta^{\mu}_{\nu} \ . \tag{1.29}$$

For example if the action is invariant (i.e. $\delta S = 0$) under the following symmetry transformation

$$\delta x^{\mu} = X^{\mu}_{\nu} \delta \omega^{\nu} \qquad \Delta \phi = \Phi_{\nu} \delta \omega^{\nu} \qquad (1.30)$$

The surface term vanishes because $\delta S = 0$ and since $\delta \omega^{\nu}$ is arbitrary

$$0 = \int_{\partial R} J^{\mu}_{\nu} d\sigma_{\mu} \delta\omega^{\nu} = \int_{R} d^{4}x \partial_{\mu} J^{\mu}_{\nu} \delta\omega^{\nu}$$
 (1.31)

$$\frac{\delta F[f(x)]}{\delta f(y)} = \lim_{\epsilon \to 0} \frac{F[f(x) + \epsilon \delta(x - y)] - F[f(x)]}{\epsilon}$$
(1.22)

and in particular

$$\frac{\delta}{\delta f(t)}f(t') = \delta(t - t') . \tag{1.23}$$

²The functional derivative of a functional is the straightforward generalisation of the ordinary derivative

with the Noether current (The infinitesimal parameter is typically factored out of the Noether current.)

$$J^{\mu}_{\nu} = \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} \Phi_{\nu} - \Theta^{\mu}_{\kappa} X^{\kappa}_{\nu} . \tag{1.32}$$

As $\delta\omega^{\mu}$ is arbitrary function and for sufficiently smooth J^{μ}_{ν} we obtain

$$\partial_{\mu}J^{\mu}_{\nu} = 0. \tag{1.33}$$

Thus we can define a conserved charge

$$Q_{\nu} = \int_{V} d^{3}x J_{\nu}^{0} \tag{1.34}$$

of the system which is conserved when integrating over the whole volume

$$\frac{dQ_{\nu}}{dt} = \int d^3x \,\partial_0 J^0_{\nu} = \int d^3x \,\partial_i J^i_{\nu} = \int d\sigma^i J^i_{\nu} = 0 , \qquad (1.35)$$

where we used the conservation of the Noether current, $\partial_{\mu}J^{\mu}_{\nu}=0$, in the second step. The last equation holds because the current has to vanish at infinity.

1.3.1 Examples

Consider $\Delta \phi = 0$ and $\delta x^{\mu} = a^{\mu}$, where a^{μ} is a translation in space-time. Noether's theorem tells us that the Noether current is

$$J^{\mu}_{\nu} = -\Theta^{\mu}_{\kappa} a^{\kappa} \tag{1.36}$$

Time-translations, $a^0 \neq 0$, $a^i = 0$ imply the conservation of energy

$$H = \int d^3x \Theta_0^0 = \int d^3x \left[\frac{\partial \mathcal{L}}{\partial(\partial_0 \phi)} \partial_0 \phi - \mathcal{L} \right]$$
 (1.37)

and spatial translations similarly imply the conservation of momentum

$$P_{i} = \int d^{3}x \Theta_{i}^{0} = \int d^{3}x \frac{\partial \mathcal{L}}{\partial(\partial_{0}\phi)} \partial_{i}\phi$$
 (1.38)

and thus we can interpret Θ^{μ}_{ν} as energy-momentum tensor.

The energy-momentum tensor as it is defined in Eq. (1.29) is not symmetric and also not unique. We may add a term $\partial_{\lambda} f^{\lambda\mu\nu}$ with $f^{\lambda\mu\nu} = -f^{\mu\lambda\nu}$, because $\partial_{\mu}\partial_{\lambda} f^{\lambda\mu\nu}$ vanishes due to f being antisymmetric in μ, λ while the derivatives are symmetric. By choosing $f^{\lambda\mu\nu}$ appropriately we obtain the canonical energy-momentum tensor

$$T^{\mu\nu} = \Theta^{\mu\nu} + \partial_{\lambda} f^{\lambda\mu\nu} \tag{1.39}$$

which is symmetric in μ, ν . The total 4-momentum of the system is the same, since

$$\int d^3x \partial_{\lambda} f^{\lambda 0\nu} = \int d^3x \partial_i f^{i0\nu} = \int d\sigma_i f^{i0\nu} = 0$$
(1.40)

irrespective of the choice of f. The last equality holds because towards infinity the fields have to sufficiently quickly go to zero, in order for the action to be normalizable and thus also any combination of the fields $\partial_i f^{i0\nu}$ has to go to zero.

1.4 Canonical quantization – free real scalar field (3)

Before moving to quantizing a scalar field let us review the quantization of the harmonic oscillator. The quantum harmonic oscillator is defined by the Lagrangian

$$L = \frac{m}{2}\dot{q}^2 - \frac{m\omega^2}{2}q^2 \tag{1.41}$$

We can directly determine the conjugate momentum, Hamiltonian and Poisson brackets using standard techniques

$$p = \frac{\partial L}{\partial \dot{q}} = m\dot{q} \tag{1.42}$$

$$H = p\dot{q} - L = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}q^2 \tag{1.43}$$

$${q,p} = 1$$
 ${p,p} = {q,q} = 0$ (1.44)

We obtain the quantum harmonic oscillator by replacing q and p by operators \hat{q} and $\hat{p} = -i\frac{d}{dq}$ and the Poisson bracket by the commutator

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\hat{q}^2 \tag{1.45}$$

$$[\hat{q}, \hat{p}] = i$$
 $[\hat{p}, \hat{p}] = [\hat{q}, \hat{q}] = 0$. (1.46)

We proceed in the analogous way for the real scalar field. The Lagrangian density for a free real scalar field, generalized momentum, Hamiltonian density and Poisson brackets are given by

$$\mathcal{L} = -\frac{1}{2}\partial_{\mu}\phi\partial^{\mu}\phi - \frac{m^2}{2}\phi^2 + \Omega_0 \tag{1.47}$$

$$\pi = \dot{\phi} \tag{1.48}$$

$$\mathcal{H} = \frac{1}{2}\pi^2 + \frac{1}{2}\nabla\phi \cdot \nabla\phi + \frac{m^2}{2}\phi^2 - \Omega_0 \tag{1.49}$$

$$\{\phi(x,t),\pi(y,t)\} = \delta^3(x-y) \qquad \{\pi(x,t),\pi(y,t)\} = \{\phi(x,t),\phi(y,t)\} = 0.$$
 (1.50)

The Hamiltonian is positive definite and thus there is no problem with negative energies. We now quantize the real scalar field and replace the field and its conjugate by hermitian operators which satisfy the canonical (equal-time) commutation relations

$$[\phi(x,t),\pi(y,t)] = i\delta^{3}(x-y) \qquad [\pi(x,t),\pi(y,t)] = [\phi(x,t),\phi(y,t)] = 0.$$
 (1.51)

Thus the coefficients a(k) in Eq. (1.7) become operators

$$\phi(x,t) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left[a(\vec{k})e^{ik_\mu x^\mu} + a^{\dagger}(\vec{k})e^{-ik_\mu x^\mu} \right]$$
 (1.52)

$$= \int \frac{d^3k}{((2\pi)^3 2\omega_k)^{1/2}} \left[a(\vec{k}) f_k(x) + a^{\dagger}(\vec{k}) f_k^*(x) \right]$$
 (1.53)

with the positive frequency (energy) solutions

$$f_k(x) = \frac{e^{ikx}}{((2\pi)^3 2\omega_k)^{1/2}}$$
 (1.54)

which form an orthonormal set

$$\int d^3x f_k^*(x) i \stackrel{\leftrightarrow}{\partial_0} f_{k'}(x) = \delta^{(3)}(\vec{k} - \vec{k}') . \tag{1.55}$$

The operators a(k) and $a^{\dagger}(k)$ satisfy the commutation relations

$$[a(k), a^{\dagger}(k')] = \int d^3x d^3y (2\pi)^3 (4\omega_k \omega_{k'})^{1/2} [(f_k^*(x, t)i \stackrel{\leftrightarrow}{\partial_0} \phi(x, t)), (\phi(y, t)i \stackrel{\leftrightarrow}{\partial_0} f_{k'}(y, t))]$$
(1.56)

$$= i(2\pi)^3 \int d^3x d^3y (4\omega_k \omega_{k'})^{1/2}$$
 (1.57)

$$\times \left(f_k^*(x,t) i \partial_0 f_{k'}(y,t) [\pi(x,t),\phi(y,t)] + i \partial_0 f_k^*(x,t) f_{k'}(y,t) [\phi(x,t),\pi(y,t)] \right)$$
(1.58)

$$= (2\pi)^3 \int d^3x (4\omega_k \omega_{k'})^{1/2} f_k^*(x,t) i \stackrel{\leftrightarrow}{\partial_0} f_{k'}(y,t)$$
 (1.59)

$$= (2\pi)^3 2\omega_k \delta^{(3)}(k - k') \tag{1.60}$$

Note that for $\vec{k} = \vec{k'}$, there is a divergence, $\delta^{(3)}(0)$. We can formulate the quantum field theory in a mathematically more rigorous way by quantizing the theory in a finite volume V. In this case, the integrals are replaced by sums and $(2\pi)^3\delta^{(3)}(0) \to V$. See the textbook "Quantum Field Theory" by Mandl and Shaw for a discussion in terms of fields quantized in a finite volume. However this breaks Lorentz invariance and for simplicity in this course we will always work with the infinite volume limit directly using formal manipulations, but keep in mind that we can always go to a finite volume to regularize the theory. Similarly we can derive the other commutation relations

$$[a(k), a(k')] = [a^{\dagger}(k), a^{\dagger}(k')] = 0.$$
 (1.61)

The operators a(k) and $a^{\dagger}(k)$ play a similar role to the ladder operators for the quantum harmonic oscillator. We define the number operator for the wave with momentum k

$$(2\pi)^3 2\omega_k \delta^3(0) N(k) = a^{\dagger}(k) a(k) . \tag{1.62}$$

The number operator N(k) satisfies the following commutation relations

$$[N(k), a^{\dagger}(k)] = a^{\dagger}(k)$$
 $[N(k), a(k)] = -a(k)$ (1.63)

which are straightforward to show, e.g. the first one follows from

$$(2\pi)^3 2\omega_k \delta^3(0)[N(k), a^{\dagger}(k)] = [a^{\dagger}(k)a(k), a^{\dagger}(k)]$$
(1.64)

$$= a^{\dagger}(k)[a(k), a^{\dagger}(k)] + [a^{\dagger}(k), a^{\dagger}(k)]a(k)$$
 (1.65)

$$= (2\pi)^3 2\omega_k \delta^3(0) a^{\dagger}(k) \tag{1.66}$$

Thus if $|n(k)\rangle$ is an eigenstate of N(k) with eigenvalue n(k) then the states $a^{\dagger} |n(k)\rangle$ and $a(k) |n(k)\rangle$ are also eigenstates of N(k) with eigenvalues n(k) + 1 and n(k) - 1 respectively. This justifies the interpretation of the operator N(k) as a particle number (density) operator for momentum k. The number operators for different momenta k commute

$$[N(k), N(k')] = 0 (1.67)$$

and thus eigenstates of the operators N(k) form a basis.

The Hamiltonian is given by

$$H = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \frac{\omega_k}{2} \left[a^{\dagger}(k)a(k) + a(k)a^{\dagger}(k) \right]$$
 (1.68)

Similar to the quantum harmonic oscillator there is a ground state energy. It gives an infinite contribution to the energy when integrating over all momenta

$$H = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \,\omega_k a^{\dagger}(k) a(k) + (\epsilon_0 - \Omega_0) V \tag{1.69}$$

where we interpreted $(2\pi)^3\delta^3(0)$ as volume V and ϵ_0V denotes the zero-point energy of all harmonic oscillators with

$$\epsilon_0 = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \omega_k \ . \tag{1.70}$$

As only energy differences matter in the absence of gravity, we can subtract the zero point energy by choosing $\Omega_0 = \epsilon_0$ and thus the Hamiltonian becomes

$$H = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \,\omega_k a^{\dagger}(k) a(k) \tag{1.71}$$

This is formally equivalent to writing all annihilation to the right of the creation operators and setting $\Omega_0 = 0$. It is denoted *normal ordering* and we define the normal ordered product of operators AB by AB:. Similarly the normal-ordered momentum is given by

$$: P_i := \int \frac{d^3k}{(2\pi)^3 2\omega_k} \ k_i a^{\dagger}(k) a(k) \ . \tag{1.72}$$

The energy is always positive given that the particle number does not become negative. This does not occur given that the norm of the states in the Hilbert space have to be non-negative. Let $|n(k)\rangle$ be a state with occupation number n(k) for momentum k, then

$$[a(k)|n(k)\rangle]^{\dagger} [a(k)|n(k)\rangle] = \left\langle n(k)|a^{\dagger}(k)a(k)|n(k)\rangle = (2\pi)^{3} 2\omega_{k} \delta^{3}(0) \left\langle n(k)|N(k)|n(k)\rangle \right\rangle$$

$$\simeq 2\omega_{k} V n(k) \left\langle n(k)|n(k)\rangle \right\rangle \geq 0 ,$$

$$(1.73)$$

where we employed the finite volume limit in the second line. Thus as a(k) reduces n(k) by 1, there is a ground state $|0\rangle$ with

$$a(k)|0\rangle = 0 \tag{1.74}$$

which does not contain any particles of momentum k. The operator a(k) and $a^{\dagger}(k)$ are commonly called annihilation and creation operators, because they annihilate and create one particle with momentum k, respectively. The vacuum expectation value of one field operator vanishes

$$\langle 0|\phi|0\rangle = 0. \tag{1.75}$$

The one-particle state $|k\rangle = a^{\dagger}(k)|0\rangle$ is normalized as

$$\langle k|k'\rangle = \langle 0|a(k)a^{\dagger}(k')|0\rangle = \langle 0|[a(k), a^{\dagger}(k')]|0\rangle = (2\pi)^3 2\omega_k \delta^3(k - k')$$
(1.76)

where we used the commutation relation³ of the creation and annihilation operators and the normalization of the vacuum state $\langle 0|0\rangle = 1$. The one-particle wave function $\psi(x)$ for a particle with momentum p is

$$\psi(x) \equiv \langle 0|\phi(x)|p\rangle = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left[\langle 0|a(k)|p\rangle e^{ikx} + \left\langle 0|a^{\dagger}(k)|p\rangle e^{-ikx} \right] = e^{ipx} . \tag{1.77}$$

1.5 Lehmann-Symanzik-Zimmermann (LSZ) reduction formula (5)

Consider a real scalar field theory. States in a free theory (i.e. which contain at most terms quadratic in the fields) are constructed by acting with the creation operators on the vacuum. A one-particle state is given by

$$|k\rangle = a^{\dagger}(k)|0\rangle \tag{1.78}$$

where the creation operator can be written in terms of the field operator as derived in Eq. (1.11)

$$a^{\dagger}(k) = \int d^3x \ e^{ikx} \left(\omega_k - i\partial_0\right) \phi(x) = -i \int d^3x \ e^{ikx} \stackrel{\leftrightarrow}{\partial_0} \phi(x)$$
 (1.79)

and similarly

$$a(k) = \int d^3x \ e^{-ikx} \left(\omega_k + i\partial_0\right) \phi(x) \ . \tag{1.80}$$

We can define the creation operator of a particle localized in momentum space near \vec{k}_1 and in position space near the origin by

$$a_1^{\dagger} = \int d^3k f_1(k) a^{\dagger}(k)$$
 (1.81)

where the function f_1 describes the wave packet of the particle, which we take to be a Gaussian with width σ

$$f_1(k) \propto \exp\left(-\frac{(\vec{k} - \vec{k_1})^2}{2\sigma^2}\right)$$
 (1.82)

In the Schrödinger picture the state $a_1^{\dagger}|0\rangle$ will propagate and spread out. The two particles in a two-particle state $a_1^{\dagger}a_2^{\dagger}|0\rangle$ with $k_1 \neq k_2$ are widely separated for $t \to \infty$. The creation and annihilation

³Note that some textbooks use a non-covariant normalization of the commutation relation $[a(k), a^{\dagger}(k')] = \delta(k - k')$.

operators are time-dependent. A suitable initial (final) state of a scattering experiment is

$$|i\rangle = \lim_{t \to -\infty} a_1^{\dagger}(t) a_2^{\dagger}(t) |0\rangle \equiv a_1^{\dagger}(-\infty) a_2^{\dagger}(-\infty) |0\rangle$$
(1.83)

$$|f\rangle = \lim_{t \to \infty} a_{1'}^{\dagger}(t)a_{2'}^{\dagger}(t)|0\rangle \equiv a_{1'}^{\dagger}(\infty)a_{2'}^{\dagger}(\infty)|0\rangle \tag{1.84}$$

The scattering amplitude is then given by $\langle f|i\rangle$. Note however that the creation and annihilation operators in the scattering amplitude are evaluated at different times. We thus have to relate them to each other.

$$a_1^{\dagger}(\infty) - a_1^{\dagger}(-\infty) = \int_{-\infty}^{\infty} dt \partial_0 a_1^{\dagger}(t)$$
 fundamental theorem of calculus (1.85)

$$= \int d^3k f_1(k) \int d^4x \partial_0 \left(e^{ikx} (\omega_k - i\partial_0) \phi(x) \right)$$
 (1.86)

$$= -i \int d^3k f_1(k) \int d^4x e^{ikx} \left(\partial_0^2 + \omega^2\right) \phi(x) \tag{1.87}$$

$$= -i \int d^3k f_1(k) \int d^4x e^{ikx} \left(\partial_0^2 + \vec{k}^2 + m^2\right) \phi(x)$$
 (1.88)

$$= -i \int d^3k f_1(k) \int d^4x e^{ikx} \left(\partial_0^2 - \stackrel{\leftarrow}{\nabla}^2 + m^2\right) \phi(x)$$
 (1.89)

$$= -i \int d^3k f_1(k) \int d^4x e^{ikx} \left(\partial_0^2 - \stackrel{\rightarrow}{\nabla}^2 + m^2\right) \phi(x)$$
 (1.90)

$$= -i \int d^3k f_1(k) \int d^4x e^{ikx} \left(-\partial_\mu \partial^\mu + m^2 \right) \phi(x) \tag{1.91}$$

and similarly for the annihilation operator

$$a_1(\infty) - a_1(-\infty) = i \int d^3k f_1(k) \int d^4x e^{-ikx} \left(-\partial_\mu \partial^\mu + m^2 \right) \phi(x)$$
 (1.92)

Thus we are in a position to evaluate the scattering amplitude, the matrix elements of the scattering operator S,

$$S_{fi} \equiv \langle f|i\rangle = \left\langle 0|T\left(a_{2'}(\infty)a_{1'}(\infty)a_{1}^{\dagger}(-\infty)a_{2}^{\dagger}(-\infty)\right)|0\rangle$$

$$= i^{4} \int d^{4}x_{1}e^{ik_{1}x_{1}}(-\partial_{1}^{2} + m^{2}) \dots d^{4}x_{2'}d^{4}x_{2'}e^{-ik_{2'}x_{2'}}(-\partial_{2'}^{2} + m^{2}) \langle 0|T\phi(x_{1})\dots\phi(x_{2'})|0\rangle$$

$$(1.93)$$

where we inserted the time-ordering operator in the first step, then used the derived relation of the creation and annihilation operators. The expression directly generalizes for more particles in the initial and/or final state. The general result is called the Lehmann-Symanzik-Zimmermann (LSZ) reduction formula, which relates the scattering amplitude to the expectation value of the time-ordered product of field operators. The same holds in an interacting theory if the fields satisfies the following two conditions

$$\langle 0|\phi(x)|0\rangle = 0 \qquad \qquad \langle 0|\phi(x)|k\rangle = e^{ikx} \,. \tag{1.94}$$

These conditions can always be satisfied by shifting and rescaling the field operator appropriately: A given field operator $\phi(x)$ can be related to the field operator at the origin via the translation $\phi(x) = e^{-iPx}\phi(0)e^{iPx}$, where P^{μ} is the energy-momentum four vector. As the vacuum is Lorentz-invariant we find

$$\langle 0|\phi(x)|0\rangle = \langle 0|e^{-iPx}\phi(0)e^{iPx}|0\rangle = \langle 0|\phi(0)|0\rangle \equiv v \tag{1.95}$$

The right-hand side is a Lorentz-invariant number. In case $v \neq 0$, we can shift the field $\phi(x) \to \phi(x) - v$ to obtain a shifted field where the first condition is satisfied. Similarly consider a one-particle state $|p\rangle$, then

$$\langle p|\phi(x)|0\rangle = \langle p|e^{-iPx}\phi(0)e^{iPx}|0\rangle = e^{-ipx}\langle p|\phi(0)|0\rangle . \tag{1.96}$$

As $\langle p|\phi(0)|0\rangle$ is a Lorentz-invariant number, which is a function of $p^2=-m^2$. We can always rescale the field $\phi(x)\to\phi(x)/\langle p|\phi(0)|0\rangle$ such that the rescaled field satisfies the second condition. The two conditions ensure that the interacting one-particle states behave like free one-particle states.

In general the creation operator will create a mixture of one-particle and multi-particle states in an interacting theory. However, it can be shown that multi-particle states separate from one-particle states at the infinite past and future and thus we can consider scattering between (quasi-)free particles: The field operator may multi-particle states $|p,n\rangle$ with total 4-momentum and a set of quantum numbers n. Following the same argument, we find

$$\langle p, n | \phi(x) | 0 \rangle = \langle p, n | e^{-iPx} \phi(0) e^{iPx} | 0 \rangle = e^{-ipx} \langle p, n | \phi(0) | 0 \rangle = e^{-ipx} A_n(\mathbf{p}) , \qquad (1.97)$$

where A_n is a function of Lorentz-invariant products of the different momenta involved in the multiparticle state. The energy of the multiparticle state satisfies $p^0 = (\vec{p}^2 + M^2)^{1/2}$ with the invariant mass $M \geq 2m$. The dispersion relation in the $(|\vec{p}|, E)$ plane contains a hyperbola for a single particle state which passes through (0, m), possibly several hyperbola for bound states passing through $|\vec{p}| = 0$ for E < 2m and a continuum of states which passes through $|\vec{p}| = 0$ with E > 2m. If $A_n(\mathbf{p})$ is non-zero, multiple particle states may be generated in the scattering which may invalidate the LSZ reduction formula. Precisely we have to ensure that $\langle p, n|a_1^{\dagger}(\pm \infty)|0\rangle = 0$ for normalizable states. Consider a general multiparticle state

$$|\psi\rangle = \sum_{n} \int d^3p \psi_n(\mathbf{p}) |p, n\rangle$$
 (1.98)

with wave functions $\psi_n(\mathbf{p})$ for the total 3-momentum \mathbf{p} . Using Eqs. (1.79), (1.81), (1.98), we obtain

$$\left\langle \psi | a_1^{\dagger}(t) | 0 \right\rangle = \sum_n \int d^3 p \psi_n^*(\vec{p}) \int d^3 k f_1(k)(-i) \int d^3 x e^{ikx} \stackrel{\leftrightarrow}{\partial_0} \left\langle p, n | \phi(x) | 0 \right\rangle \tag{1.99}$$

$$= -i\sum_{n} \int d^3p \psi_n^*(\vec{p}) \int d^3k f_1(k) \int d^3x (e^{ikx} \stackrel{\leftrightarrow}{\partial_0} e^{-ipx}) A_n(\mathbf{p})$$
 (1.100)

$$= \sum_{n} \int d^{3}p \psi_{n}^{*}(\vec{p}) \int d^{3}k f_{1}(k) \int d^{3}x (p^{0} + k^{0}) e^{i(k-p)x} A_{n}(\mathbf{p})$$
(1.101)

$$= \sum_{n} \int d^{3}p \psi_{n}^{*}(\vec{p}) \int d^{3}k f_{1}(k) (p^{0} + k^{0}) (2\pi)^{3} \delta^{(3)}(\vec{k} - \vec{p}) e^{i(p^{0} - k^{0})t} A_{n}(\mathbf{p})$$
(1.102)

with $p_0 = (\bar{p}^2 + M^2)^{1/2}$ and $k^0 = (\bar{p}^2 + m^2)^{1/2} < p^0$. We used Eq. (1.97) in the second line, evaluated the time derivative in the third line, integrated over x in the fourth line.

The final step is to evaluated the d^3k integral and to use the Riemann-Lebesgue lemma.⁴

$$\left\langle \psi | a_1^{\dagger}(t) | 0 \right\rangle = (2\pi)^3 \sum_n \int d^3 p \psi_n^*(\vec{p}) f_1(p) (p^0 + k^0) e^{i(p^0 - k^0)t} A_n(\mathbf{p}) \stackrel{t \to \pm \infty}{\longrightarrow} 0 \tag{1.103}$$

This relies on the assumption that the wave functions are normalizable. See the discussion in the book by Mark Srednicki and arXiv:1904.10923 [hep-ph] for more details. Next we develop tools to calculate correlation functions such as $\langle 0|T\phi(x_1)\dots\phi(x_n)|0\rangle$.

⁴The Riemann-Lebesgue lemma states that for L^1 integrable functions, i.e. $\int |f| dx$ is finite, the Fourier transform of f satisfies $\int f(x)e^{-izx} dx \to 0$ for $|z| \to 0$.

2 Feynman path integral

2.1 Derivation (6, Weinberg)

We develop the formulation of a quantum theory in terms of the Feynman path integral. Consider the generalized coordinate operators Q_a and their conjugate momentum operators P_a with the canonical commutation relations

$$[Q_a, P_b] = i\delta_{ab}$$
 $[Q_a, Q_b] = [P_a, P_b] = 0$ (2.1)

In a field theory the operators depend on the position x. Thus the index a labels on the one hand the position x and on the other hand a discrete species index m. Thus the Kronecker delta function δ_{ab} should be interpreted as $\delta_{x,m;y,n} = \delta(x-y)\delta_{m,n}$. As the Q_a (P_a) commute among each other there are simultaneous eigenstates $|q\rangle$ $(|p\rangle)$ with eigenvalues q_a (p_a)

$$Q_a |q\rangle = q_a |q\rangle$$
 $P_a |p\rangle = p_a |p\rangle$ (2.2)

which are orthogonal and satisfy a completeness relation

$$\langle q'|q\rangle = \Pi_a \delta(q'_a - q_a) \equiv \delta(q' - q)$$
 $\langle p'|p\rangle = \Pi_a \delta(p'_a - p_a) \equiv \delta(p' - p)$ (2.3)

$$1 = \int \Pi_a dq_a |q\rangle \langle q| \equiv \int d\underline{q} |q\rangle \langle q| \qquad \qquad 1 = \int \Pi_a dp_a |p\rangle \langle p| \equiv \int d\underline{p} |p\rangle \langle p| \qquad (2.4)$$

From the commutation relations (2.1) the scalar product

$$\langle q|p\rangle = \Pi_a \frac{1}{\sqrt{2\pi}} e^{iq_a p_a} \tag{2.5}$$

follows. In the Heisenberg picture⁵ the operators P_a and Q_a depend on time

$$Q_a(t) = e^{iHt}Q_ae^{-iHt} P_a(t) = e^{iHt}P_ae^{-iHt} (2.7)$$

and thus the eigenstates of Q(t) (P(t)) and Q(P) are related by

$$|q;t\rangle = e^{iHt}|q\rangle$$
 $|p;t\rangle = e^{iHt}|p\rangle$ (2.8)

The corresponding completeness and orthogonality relations apply

$$\langle q'; t|q; t \rangle = \Pi_a \delta(q'_a - q) \equiv \delta(q' - q)$$
 $\langle p'; t|p; t \rangle = \Pi_a \delta(p'_a - p) \equiv \delta(p' - p)$ (2.9)

$$1 = \int d\underline{q} |q; t\rangle \langle q; t| = \int d\underline{p} |p; t\rangle \langle p; t| \qquad \langle q; t| p; t\rangle = \Pi_a \frac{1}{\sqrt{2\pi}} e^{iq_a p_a} . \qquad (2.10)$$

$$|a;t\rangle_H = e^{iHt} |a\rangle_S$$

$$A_H(t) = e^{iHt} A_S e^{-iHt}.$$
 (2.6)

⁵States $|a\rangle$ and operators A in the Heisenberg picture are related to operators in the "Schödinger picture at fixed time t=0" by

Now we want to calculate the probability amplitude for a system to go from state $|q;t\rangle$ to state $|q';t'\rangle$, i.e. the scalar product $\langle q';t'|q;t\rangle$. For an infinitesimally small time difference dt=t'-t, it is given by

$$\left\langle q';t'|q;t\right\rangle = \left\langle q';t|e^{-iH(Q(t),P(t))dt}|q;t\right\rangle = \int d\underline{p}\left\langle q';t|e^{-iH(Q(t),P(t))dt}|p;t\right\rangle \left\langle p;t|q;t\right\rangle \tag{2.11}$$

$$= \int \Pi_a \frac{dp_a}{2\pi} e^{-iH(q',p)dt + i\sum_a (q'_a - q_a)p_a}$$
 (2.12)

The last step is only possible for an infinitesimal time step, where $\exp(-iHdt) \simeq 1 - iHdt$, because we can neglect higher orders in dt. For a finite time interval, we split the the time interval in many intermediate steps, $t \equiv \tau_0, \tau_1, \tau_2, \dots, \tau_N, \tau_{N+1} \equiv t'$ with $\tau_{k+1} - \tau_k = \delta \tau = (t'-t)/(N+1)$ and insert the identity using the completeness relation for the states q. Hence the scalar product is given by the constrained⁷ path integral

$$\langle q'; t'|q; t \rangle = \int \prod_{k=1}^{N} d\underline{q}(\tau_{k}) \langle q(\tau_{N+1}); \tau_{N+1}|q(\tau_{N}); \tau_{N} \rangle \langle q(\tau_{N}); \tau_{N}|q(\tau_{N-1}); \tau_{N-1} \rangle \dots \langle q(\tau_{1}); \tau_{1}|q(\tau_{0}); \tau_{0} \rangle$$

$$= \int \left[\prod_{k=1}^{N} d\underline{q}(\tau_{k}) \right] \left[\prod_{k=0}^{N} \prod_{a} \frac{dp_{k,a}}{2\pi} \right]$$

$$\times \exp \left(i \sum_{k=1}^{N+1} \left[\sum_{a} (q_{a}(\tau_{k}) - q_{a}(\tau_{k-1})) p_{a}(\tau_{k-1}) - H(q(\tau_{k}), p(\tau_{k-1})) d\tau \right] \right)$$

$$\stackrel{N \to \infty}{\longrightarrow} \int_{q(t^{(\prime)}) = q^{(\prime)}} \mathcal{D}q \mathcal{D}p \exp \left(i \int_{t}^{t'} \left[\sum_{a} \dot{q}_{a}(\tau) p_{a}(\tau) - H(q(\tau), p(\tau)) \right] d\tau \right)$$

$$(2.14)$$

where we implicitly defined the integration measure

$$\int \mathcal{D}q\mathcal{D}p = \lim_{N \to \infty} \int \left[\Pi_{k=1}^N \Pi_a dq_a(\tau_k) \right] \left[\Pi_{k=0}^N \Pi_a \frac{dp_a(\tau_k)}{2\pi} \right] . \tag{2.15}$$

Note that q and p in the path integral are ordinary functions (instead of operators). They are variables of integration and do not generally satisfy the classical Hamiltonian dynamics. For convenience we define the function

$$S = \int_{t}^{t'} d\tau \left[\dot{q}(\tau)p(\tau) - H \right] , \qquad (2.16)$$

which reduces to the action if the Hamiltonian dynamics holds.

2.2 Expectation values of operators (6, Weinberg)

The Feynman path integral formalism allows to calculate expectation values of operators for intermediate times. Consider an operator⁸ $O(t_1)$ at time t_1 with $t < t_1 < t'$. For an infinitesimal time interval

⁶The Hamiltonian is a function of the operators Q and P. In the Heisenberg picture, it is given by the same function of Q(t) and P(t). We adopt a standard-form of the Hamiltonian where all operators Q appear to the left of the operators P. Other conventions are possible (e.g. Weyl ordering) but will lead to slight differences in the definition of the Feynman path integral.

⁷The initial and final state are fixed and not varied.

⁸The operators Q_a have to be ordered to the right of the conjugate operators P_a .

[t, t + dt] with an insertion of an operator at time t we find

$$\langle q'; t + dt | O(P(t), Q(t)) | q; t \rangle = \int \Pi_a \frac{dp_a}{2\pi} \left\langle q'; t | e^{-iH(Q(\tau), P(\tau))dt} | p; t \right\rangle \langle p; t | O(P(t), Q(t)) | q; t \rangle \quad (2.17)$$

$$= \int \Pi_a \frac{dp_a}{2\pi} O(p, q) e^{-iH(q', p)dt + i\sum_a (q'_a - q_a)p_a} , \quad (2.18)$$

i.e. for every operator we insert the operator with Q and P replaced by the integration variables q and p, respectively. Thus for a finite time interval $t < t_1 < t'$ we simply obtain

$$\langle q'; t'|O(P(t_1), Q(t_1))|q; t\rangle = \int \mathcal{D}q \mathcal{D}p \ O(p(t_1), q(t_1))e^{iS} \ . \tag{2.19}$$

Then its expectation value can be expressed in terms of a path integral. Similarly for multiple operators $O_1(t_1)$ and $O_2(t_2)$

$$\int \mathcal{D}q \mathcal{D}p \ O_1(p(t_1), q(t_1)) O_2(p(t_2), q(t_2)) e^{iS} = \begin{cases} \langle q'; t' | O_2(P(t_2), Q(t_2)) O_1(P(t_1), Q(t_1)) | q; t \rangle & t_1 < t_2 \\ \langle q'; t' | O_1(P(t_1), Q(t_1)) O_2(P(t_2), Q(t_2)) | q; t \rangle & t_2 < t_1 \end{cases}$$
(2.20)

The right-hand side can be expressed in terms of the time-ordered product of the operators

$$TO(t_1)O(t_2) = \begin{cases} O(t_1)O(t_2) & t_2 < t_1 \\ O(t_2)O(t_1) & t_1 < t_2 \end{cases}$$
 (2.21)

It straightforwardly generalizes to the time-ordered product of an arbitrary number of operators.

$$\langle q'; t'|TO_1(t_1)\dots O_n(t_n)|q;t\rangle = \int \mathcal{D}q\mathcal{D}pO_1(t_1)\dots O_n(t_n)e^{iS}$$
 (2.22)

This motivates the introduction of external sources J and K for a particle in quantum mechanics (field in quantum field theory)

$$\langle q'; t'|q; t\rangle_{J,K} = \int \mathcal{D}q \mathcal{D}p e^{i(S+Jq+Kp)}$$
 (2.23)

where the products Jq and Kp should be understood as $Jq = \int d\tau J(\tau)q(\tau)$. Functional derivatives (See footnote 2) with respect to the external sources evaluated for vanishing external sources then generates the time-ordered product of the corresponding operators. For example there is

$$\frac{1}{i} \frac{\delta}{\delta J(t_1)} \left\langle q'; t' | q; t \right\rangle_{J,K} \bigg|_{J=K=0} = \int \mathcal{D}q \mathcal{D}p q(t_1) e^{iS} = \left\langle q'; t' | Q(t_1) | q; t \right\rangle \tag{2.24}$$

$$\frac{1}{i} \frac{\delta}{\delta K(t_1)} \left\langle q'; t' | q; t \right\rangle_{J,K} \bigg|_{J=K=0} = \int \mathcal{D}q \mathcal{D}p p(t_1) e^{iS} = \left\langle q'; t' | P(t_1) | q; t \right\rangle \tag{2.25}$$

$$\frac{1}{i} \frac{\delta}{\delta J(t_2)} \frac{1}{i} \frac{\delta}{\delta J(t_1)} \left\langle q'; t' | q; t \right\rangle_{J,K} \bigg|_{J=K=0} = \int \mathcal{D}q \mathcal{D}pq(t_1) q(t_2) e^{iS} = \left\langle q'; t' | TQ(t_1)Q(t_2) | q; t \right\rangle \tag{2.26}$$

and in general

$$\frac{1}{i} \frac{\delta}{\delta J(t_1)} \dots \frac{1}{i} \frac{\delta}{\delta K(t_n)} \left\langle q'; t' | q; t \right\rangle_{J,K} \bigg|_{I=K=0} = \left\langle q'; t' | TQ(t_1) \dots P(t_n) \dots | q; t \right\rangle. \tag{2.27}$$

2.3 Vacuum-vacuum transition (6, Weinberg)

So far we only considered position eigenstates as initial and final states. For other initial and final states we have to multiply with the wave functions $\langle q|\phi\rangle=\phi(q)$ of these states and integrate over the generalized positions. In particular if we consider transition amplitudes from the infinite past to the infinite future

$$\langle \phi; \infty | \psi; -\infty \rangle_{J,K} = \int dq' dq \int_{q(\infty) = q', q(-\infty) = q} \mathcal{D}\underline{q} \mathcal{D}\underline{p} \phi^*(q(\infty)) \psi(q(-\infty)) e^{i(S + Jq + Kp)}$$
(2.28)

$$= \int \mathcal{D}\underline{q}\mathcal{D}\underline{p}\phi^*(q(\infty))\psi(q(-\infty))e^{i(S+Jq+Kp)}$$
(2.29)

where we used that the unconstrained Feynman path integral is equivalent to the constrained path integral when we integrate over the boundary conditions. An analogous expression holds for the expectation value of operators.

As discussed in the derivation of the LSZ reduction formula we are specifically interested in vacuum to vacuum transition amplitudes

$$\langle 0; \infty | 0; -\infty \rangle_{J,K} = \int \mathcal{D}\underline{q} \mathcal{D}\underline{p} \ e^{i(S+Jq+Kp)} \langle 0; \text{out} | q(\infty); \infty \rangle \langle q(-\infty); -\infty | 0; \text{in} \rangle$$
 (2.30)

Thus we have to evaluate the ground state wave functions in the infinite past and future. We consider two concrete simple examples of free field theories, a quantum theory which reduces to the quantum harmonic oscillator in the absence of interactions and a real scalar field, but before discussing them we first introduce the Lagrangian version of the path integral.

2.4 Lagrangian version (6, Weinberg)

In case the Hamiltonian is quadratic in the conjugate momenta it is a Gaussian integral and the integral over the conjugate momenta can be performed exactly. If additionally the quadratic term in the conjugate momenta does not depend on the generalized variables q the result will only involve constants which can be absorbed in the definition of the integration measure

$$\langle q'; t'|q; t \rangle = \int_{q(t^{(\prime)})=q^{(\prime)}} \mathcal{D}q \exp\left(i \int_t^{t'} d\tau L(q(\tau), \dot{q}(\tau))\right)$$
 (2.32)

The function $L(\dot{q},q)$ is computed by first determining the stationary point, i.e. by solving

$$0 = \frac{\delta}{\delta p_a(\tau)} \left(\int_t^{t'} \left[\sum_a \dot{q}_a(\tau') p_a(\tau') - H(q(\tau'), p(\tau')) \right] d\tau' \right) = \dot{q}_a(\tau) - \frac{\partial H(q(\tau), p(\tau))}{\partial p_a(\tau)}$$
(2.33)

$$\int dx e^{-(\frac{1}{2}xAx + bx + c)} = \int dx' e^{-(\frac{1}{2}x'Ax' + c - \frac{1}{2}bA^{-1}b)} = \sqrt{\frac{2\pi}{A}} e^{\frac{1}{2}bA^{-1}b - c}$$
(2.31)

with $x' = x + A^{-1}b$.

⁹Note that the Gaussian integral is simply

for p in terms of q and \dot{q} , and then inserting the solution in integrand. This exactly mirrors the procedure in classical mechanics, when we move from the Hamiltonian formulation to Lagrangian formulation. The function L is the Lagrangian of the system. In the Lagrangian formulation the path integral is explicitly Lorentz invariant. This situation is very common and in particular it applies for the theories we are interested in for the rest of the lecture. Thus we will mostly use the Lagrangian version in the following.

2.5 Quantum harmonic oscillator (7)

The Hamiltonian and the Lagrangian of the harmonic oscillator take the form

$$H = \frac{p^2}{2} + \frac{1}{2}\omega^2 q^2 \qquad L = \frac{1}{2}\dot{q}^2 - \frac{1}{2}\omega^2 q^2$$
 (2.34)

using convenient units where m=1. The relevant commutation relations are

$$[p,q] = -i$$
 $[p,p] = [q,q] = 0$ (2.35)

and the annihilation operator is defined by

$$a = \sqrt{\frac{\omega}{2}} \left(q + i \frac{p}{\omega} \right) . \tag{2.36}$$

In position space the momentum operator is represented by $p = -i\partial/\partial q$. Then the ground state wave function is determined by (a|0) = 0 in position space)

$$0 = \left[\omega q + \frac{\partial}{\partial q}\right] \langle q|0\rangle \qquad \Rightarrow \qquad \langle q|0\rangle = Ne^{-\frac{1}{2}\omega q^2} \tag{2.37}$$

with some normalization constant N. In particular this expression holds for the wave function in the infinite future and past and thus the product of the two wave functions is given by.

$$\langle 0; \operatorname{out}|q(\infty); \infty \rangle \langle q(-\infty); -\infty|0; \operatorname{in} \rangle = |N|^2 e^{-\frac{1}{2}\omega \left[q(-\infty)^2 + q(\infty)^2\right]}$$
(2.38)

$$= \lim_{\epsilon \to 0^+} |N|^2 e^{-\frac{\epsilon}{2}\omega \int_{-\infty}^{\infty} d\tau q(\tau)^2 e^{-\epsilon|\tau|}}$$
 (2.39)

where we used the final value theorem of the Laplace transform. Note that the wave function is independent of the sources and thus only contributes a constant factor to the Feynman path integral. As we are only interested in the limit $\epsilon \to 0$ (and $q(\tau)^2$ is integrable for the harmonic oscillator), this motivates the definition of the partition function

$$Z[J,K] = \langle 0; \infty | 0; -\infty \rangle_{J,K} = \frac{\lim_{\epsilon \to 0} \int \mathcal{D}\underline{q} \mathcal{D}\underline{p} \, e^{i(S+Jq+Kp+i\epsilon \int d\tau \frac{1}{2}q^2)}}{\lim_{\epsilon \to 0} \int \mathcal{D}\underline{q} \mathcal{D}\underline{p} \, e^{i(S+i\epsilon \int d\tau \frac{1}{2}q^2)}}$$
(2.40)

as a generating functional of all correlation functions for vacuum to vacuum transitions. The correlation functions are obtained by taking derivatives with respect to the sources of Z[J, K]. Equivalently we could discard the normalization factor and consider $\ln Z[J, K]$, because derivatives of $\ln Z[J, K]$ are

automatically correctly normalized such that vacuum-vacuum transition amplitude in the absence of sources is normalized to unity, i.e. $\langle 0|0\rangle_{J=K=0}=1$. Similarly the partition function in the Lagrangian formulation is given by

$$Z[J] = \frac{\lim_{\epsilon \to 0} \int \mathcal{D}\underline{q} \ e^{i(S+Jq+i\epsilon \int d\tau \frac{1}{2}q^2)}}{\lim_{\epsilon \to 0} \int \mathcal{D}q \ e^{i(S+i\epsilon \int d\tau \frac{1}{2}q^2)}} \ . \tag{2.41}$$

It is convenient to consider the Fourier-transform of q

$$\tilde{q}(E) = \int dt e^{iEt} q(t) \qquad q(t) = \int \frac{dE}{2\pi} e^{-iEt} \tilde{q}(E) \qquad (2.42)$$

and equivalently for the source J(t). Thus the term in the exponent becomes

$$S + Jq + \int \frac{i\epsilon}{2} q(\tau)^2 = \frac{1}{2} \int d\tau \frac{dE}{2\pi} \frac{dE'}{2\pi} e^{-i(E+E')\tau} \left[\left(-EE' - \omega^2 + i\epsilon \right) \tilde{q}(E) \tilde{q}(E') + \tilde{J}(E) \tilde{q}(E') + \tilde{J}(E') \tilde{q}(E) \right]$$
$$= \frac{1}{2} \int \frac{dE}{2\pi} \left[\tilde{q}(E) \left(E^2 - \omega^2 + i\epsilon \right) \tilde{q}(-E) + \tilde{J}(E) \tilde{q}(-E) + \tilde{J}(-E) \tilde{q}(E) \right]$$
(2.43)

where we used that the τ -integration yields a factor $2\pi\delta(E+E')$ which has been used to perform the E'-integration. The path integral measure is invariant under a shift of the integration variables, $\tilde{q}(E) \to \tilde{q}(E) - \frac{J(E)}{E^2 - \omega^2 + i\epsilon}$ and thus the amplitude is given by

$$Z[J] = \frac{1}{Z[0]} \exp\left(\frac{i}{2} \int \frac{dE}{2\pi} \frac{\tilde{J}(E)\tilde{J}(-E)}{-E^2 + \omega^2 - i\epsilon}\right) \times \int \mathcal{D}\underline{\tilde{q}} \exp\left(\frac{i}{2} \int \frac{dE}{2\pi} \tilde{q}(E) \left[E^2 - \omega^2 + i\epsilon\right] \tilde{q}(-E)\right)$$
(2.44)

$$= \exp\left(\frac{i}{2} \int \frac{dE}{2\pi} \frac{\tilde{J}(E)\tilde{J}(-E)}{-E^2 + \omega^2 - i\epsilon}\right). \tag{2.45}$$

Taking an inverse Fourier transform we obtain

$$Z[J] = \exp\left(\frac{i}{2} \int dt dt' J(t) G(t - t') J(t')\right)$$
(2.46)

The Fourier transform of the kernel

$$G(t - t') \equiv \int \frac{dE}{2\pi} \frac{e^{-iE(t - t')}}{-E^2 + \omega^2 - i\epsilon}$$
(2.47)

is a Green's function of the harmonic oscillator

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2\right) G(t - t') = \delta(t - t') \tag{2.48}$$

which can be shown by a straightforward calculation of the left-hand side. The integral over the energy E in the definition of the Green's function can also be evaluated via a contour integral in the complex E plane via the residue theorem.¹⁰ The two simple poles are at $E = \pm (\omega - i\epsilon)$, i.e. the pole

$$\oint_{\gamma} f(z)dz = 2\pi i \sum_{k} \operatorname{Res}(f, a_{k}). \tag{2.49}$$

¹⁰The residue theorem relates the contour integral along a positively oriented simple closed curve to the sum of the residues of the enclosed poles

for positive (negative) energy is shifted slightly to the lower (upper) half of the complex plane. For t - t' > 0 (t - t' < 0) we close the contour via the lower (upper) half of the complex plane and thus the residue theorem results in

$$G(t - t') = \frac{i}{2\omega} e^{-i\omega|t - t'|}. \tag{2.51}$$

The Green's function can similarly be expressed in terms of the 2-point correlation function. The second derivative with respect to the sources of the partition function is

$$\langle 0|TQ(t_1)Q(t_2)|0\rangle = \frac{1}{i} \frac{\delta}{\delta J(t_1)} \frac{1}{i} \frac{\delta}{\delta J(t_2)} Z[J] \Big|_{J=0} = \frac{1}{i} \frac{\delta}{\delta J(t_1)} \left[\int dt' G(t_2 - t') J(t') \right] Z[J] \Big|_{J=0}$$
(2.52)
$$= \frac{1}{i} G(t_2 - t_1) .$$
(2.53)

We can similarly evaluate higher-order correlation functions. For the four-point function we find

$$\langle 0|TQ(t_1)Q(t_2)Q(t_3)Q(t_4)|0\rangle = \frac{1}{i^2} \left[G(t_2 - t_1)G(t_4 - t_3) + G(t_3 - t_1)G(t_4 - t_2) + G(t_4 - t_1)G(t_3 - t_2) \right] . \tag{2.54}$$

Thus the 4-point correlation function is given by the sum of the Green's functions of all possible pairings. More generally 2n-point function is given by

$$\langle 0|TQ(t_1)\dots Q(t_{2n})|0\rangle = \frac{1}{i^n} \sum_{\text{pairings}} G(t_{i_1} - t_{i_2})\dots G(t_{i_{2n-1}} - t_{i_{2n}}).$$
 (2.55)

All other n-point functions, i.e. with odd n vanish, because there is always one remaining source term. Interactions from terms in the Lagrangian with higher powers of the generalized coordinate q^n , n > 2 will change this result.

2.6 Free scalar field (8)

Next, we are looking at a free scalar field. The Lagrangian density is given by

$$\mathcal{L} = -\frac{1}{2}\partial_{\mu}\phi\partial^{\mu}\phi - \frac{m^2}{2}\phi^2 \tag{2.56}$$

The derivation of the $i\epsilon$ factor proceeds in the same way as for harmonic oscillator. The correct prescription is obtained by adding a term $+i\epsilon \frac{1}{2}\phi^2$ to the Lagrangian. Details are presented in Sec. 3.5. The generating functional is then given by

$$Z[J] = \frac{\int \mathcal{D}\phi \exp\left(i \int d^4x \left(\mathcal{L} + J(x)\phi(x)\right)\right)}{\int \mathcal{D}\phi \exp\left(i \int d^4x \mathcal{L}\right)}$$
(2.57)

$$= \frac{\int \mathcal{D}\phi \exp\left(-\frac{i}{2} \int d^4x d^4x' \phi(x) \phi(x') D(x, x') + i \int d^4x J(x) \phi(x)\right)}{\int \mathcal{D}\phi \exp\left(-\frac{i}{2} \int d^4x d^4x' \phi(x) \phi(x') D(x, x')\right)}$$
(2.58)

In particular for a holomorphic function f the Cauchy integral theorem states

$$2\pi i f(a) = \oint_{\gamma} dz \frac{f(z)}{z - a} . \tag{2.50}$$

where D(x, y) in the second line is defined as

$$D(x,x') = \left[\frac{\partial}{\partial x'_{\mu}} \frac{\partial}{\partial x^{\mu}} + m^2 - i\epsilon\right] \delta(x-x')$$
 (2.59)

which is translation invariant. In momentum space with

$$\tilde{\phi}(p) = \int d^4x e^{-ipx} \phi(x) \qquad \qquad \phi(x) = \int \frac{d^4p}{(2\pi)^4} e^{ipx} \tilde{\phi}(p)$$
 (2.60)

we thus obtain

$$\tilde{D}(p) = p^2 + m^2 - i\epsilon \tag{2.61}$$

$$S + J\phi + i\epsilon \text{ terms} = \frac{1}{2} \int \frac{d^4p}{(2\pi)^4} \left(-\tilde{\phi}(p)\tilde{D}(p)\tilde{\phi}(-p) + \tilde{J}(p)\tilde{\phi}(-p) + \tilde{J}(-p)\tilde{\phi}(p) \right)$$
(2.62)

Analogously to the derivation in case of the quantum harmonic oscillator the d^4x integration yields a factor $(2\pi)^4 \delta^{(4)}(p+p')$ which introduces the different signs for the momenta. Note that $\tilde{D}(p)$ is symmetric, $\tilde{D}(p) = \tilde{D}(-p)$ and thus using linearity of the path integral measure by shifting the field $\tilde{\phi}(p) \to \tilde{\phi}(p) + \tilde{D}(p)^{-1}\tilde{J}(p)$ we obtain

$$Z[J] = \frac{1}{Z[0]} \exp\left(-\frac{i}{2} \int \frac{d^4p}{(2\pi)^4} \tilde{J}(p)\tilde{D}(p)^{-1} \tilde{J}(-p)\right) \times \int \mathcal{D}\phi \exp\left(-\frac{i}{2} \int \frac{d^4p}{(2\pi)^4} \tilde{\phi}(p)\tilde{D}(p)\tilde{\phi}(-p)\right)$$
(2.63)

$$= \exp\left(-\frac{i}{2} \int \frac{d^4 p}{(2\pi)^4} \tilde{J}(p)\tilde{D}(p)^{-1} \tilde{J}(-p)\right)$$
 (2.64)

In position space we obtain

$$Z[J] = \exp\left(-\frac{i}{2} \int d^4x d^4x' J(x) \Delta_F(x - x') J(x')\right)$$
(2.65)

where we implicitly defined the Feynman propagator

$$\Delta_F(x - x') \equiv \int \frac{d^4p}{(2\pi)^4} \frac{e^{ip(x - x')}}{p^2 + m^2 - i\epsilon} \,. \tag{2.66}$$

The Feynman propagator is a Green's function of the Klein-Gordon equation and thus satisfies (in the limit $\epsilon \to 0$)

$$(-\Box_x + m^2) \,\Delta_F(x - x') = \delta^{(4)}(x - x') \tag{2.67}$$

which follows directly from its definition. In the complex plane of the energy there are two simple poles at $\pm \sqrt{\vec{p}^2 + m^2 - i\epsilon}$. Using the residue theorem we can evaluate the integral over the energy and obtain

$$\Delta_F(x - x') = i \int \frac{d^3p}{(2\pi)^3 2E(p)} e^{-i\omega_p |t - t'| + i\vec{p}(\vec{x} - \vec{x}')}$$
(2.68)

$$= i \theta(t - t') \int \frac{d^3p}{(2\pi)^3 2\omega_p} e^{ip(x - x')} + i\theta(t' - t) \int \frac{d^3p}{(2\pi)^3 2\omega_p} e^{ip(x' - x)}$$
(2.69)

using the result from the same calculation for the harmonic oscillator. The two remaining integrals can be evaluated in terms of modified Bessel functions which we will see when looking at the spin-statistics connection theorem. Finally analogously to the discussion for the harmonic oscillator we obtain the expectation values of the time-ordered products by taking functional derivatives with respect to the sources

$$\langle 0|T\phi(x_1)\dots\phi(x_n)|0\rangle = \frac{1}{i}\frac{\delta}{\delta J(x_1)}\dots\frac{1}{i}\frac{\delta}{\delta J(x_n)}Z[J]\bigg|_{J=0}$$
(2.70)

In particular the 2-point correlation function is given in terms of the Feynman propagator

$$\langle 0|T\phi(x_1)\phi(x_2)|0\rangle = \frac{1}{i}\Delta_F(x_2 - x_1)$$
 (2.71)

or explicitly writing out the time-ordered product we find

$$\frac{1}{i}\Delta_F(x_2 - x_1) = \theta(t_1 - t_2)\langle 0|\phi(x_1)\phi(x_2)|0\rangle + \theta(t_2 - t_1)\langle 0|\phi(x_2)\phi(x_1)|0\rangle$$
(2.72)

$$= \theta(t_1 - t_2) \langle 0|\phi^+(x_1)\phi^-(x_2)|0\rangle + \theta(t_2 - t_1) \langle 0|\phi^+(x_2)\phi^-(x_1)|0\rangle . \tag{2.73}$$

with the positive and negative frequency solutions

$$\phi^{+}(x,t) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} a(k)e^{ikx}$$
 (2.74)

$$\phi^{-}(x,t) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} a^{\dagger}(k) e^{-ikx} . \qquad (2.75)$$

Thus the Feynman propagator for $t_2 < t_1$ can be interpreted as the creation of a particle at x_2 and the annihilation of a particle at x_1 and vice versa for $t_1 < t_2$. The time-ordered product of 2n field operators is given by the sum over all pairings

$$\langle 0|T\phi(x_1)\dots\phi(x_{2n})|0\rangle = \frac{1}{i^n} \sum_{\text{pairings}} \Delta_F(x_{i_1} - x_{i_2})\dots\Delta_F(x_{i_{2n-1}} - x_{i_{2n}}).$$
 (2.76)

This result is known as Wick's theorem.

2.7 Interacting scalar field theory (9)

Finally we will be considering interactions. Consider a Lagrangian $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$ where \mathcal{L}_0 is the Lagrangian of a free field (or exactly solvable) and \mathcal{L}_1 denotes the interaction Lagrangian.¹¹ Then the generating functional can be written as

$$Z[J] = \frac{\int \mathcal{D}\phi e^{i \int d^4x \left(\mathcal{L}_0 + \mathcal{L}_1 + J\phi + i\frac{\epsilon}{2}\phi^2\right)}}{\int \mathcal{D}\phi e^{i \int d^4x \left(\mathcal{L}_0 + \mathcal{L}_1 + i\frac{\epsilon}{2}\phi^2\right)}}$$
(2.77)

 $^{^{11}}$ Recall that we made several assumptions when going to the Lagrangian formulation: H is no more than quadratic in the conjugate momenta and this term does not depend on the generalized coordinates. If this is not satisfied or if we want to calculate expectation values of conjugate momenta, we have to resort to the Hamiltonian formulation.

We are going to use our solution for the free field theory to obtain a more convenient expression for the interacting theory¹²

$$Z[J] \propto \int \mathcal{D}\phi e^{i \int d^4x \mathcal{L}_1} e^{i \int d^4x \left(\mathcal{L}_0 + J\phi + i\frac{\epsilon}{2}\phi^2\right)} = \exp\left[i \int d^4x \mathcal{L}_1\left(\frac{1}{i}\frac{\delta}{\delta J(x)}\right)\right] Z_0[J]$$
 (2.78)

with the generating functional of the free theory

$$Z_0[J] = \exp\left(\frac{i}{2} \int d^4x d^4x' J(x) \Delta_F(x - x') J(x')\right)$$
(2.79)

Thus vacuum expectation values of time-ordered products of operators are given by

$$\langle 0|T\phi(x_1)\dots\phi(x_n)|0\rangle = \frac{1}{Z[0]} \left[\frac{1}{i} \frac{\delta}{\delta J(x_1)} \dots \frac{1}{i} \frac{\delta}{\delta J(x_n)} \exp\left[i \int d^4x \mathcal{L}_1\left(\frac{1}{i} \frac{\delta}{\delta J(x)}\right) \right] Z_0[J] \right|_{J=0} . \quad (2.80)$$

In order to better understand the expression we will do a double expansion of the generating functional in terms of the number of interactions and the number of propagators Δ_F . For concreteness we will consider the simplest interaction Lagrangian

$$\mathcal{L}_1 = \frac{1}{3!} g \phi^3 \ . \tag{2.81}$$

This theory is not bounded from below and thus there is no ground state (similar to the harmonic oscillator with a q^3 correction). This however does not become obvious in perturbation theory, when we expand in the small coupling g. We will ignore it in the following and illustrate the perturbative expansion of the generating functional. The expansion of Eq. (2.78) then results in

$$Z[J] \propto \sum_{V=0}^{\infty} \frac{1}{V!} \left[\frac{ig}{6} \int d^4x \left(\frac{1}{i} \frac{\delta}{\delta J(x)} \right)^3 \right]^V \sum_{P=0}^{\infty} \frac{1}{P!} \left[\frac{i}{2} \int d^4x d^4x' J(x) \Delta_F(x - x') J(x') \right]^P . \tag{2.82}$$

For a given term in the expansion with P propagators and V vertices the number of surviving sources is E = 2P - 3V, where E stands for external legs. In case of the expectation value of a time-ordered product E has to match the number of operators in the time-ordered product. The overall phase factor of each term is $i^V \frac{1}{i^3V} i^P = i^{P-2V}$. There are several identical terms for a given set of (V, P, E), because the functional derivatives can act on the propagators in different combinations. We can represent each term in the expansion diagrammatically. The diagrams are called Feynman diagrams which have been first introduced by R. Feynman. We represent each propagator by a line and each interaction by a vertex where three lines meet. For example there is one connected 13 diagram with E = 0 and V = 0 as shown in Fig. 1 and there are 2 connected diagrams with E = 0 and V = 0 as shown in Fig. 2. The multiplicity of each diagram can be obtained by the following considerations: (i) we can rearrange the three functional derivatives of each vertex without changing the diagram. This results in a factor 3! for each vertex. (ii) We can similarly rearrange the vertices which results in a factor V!.

 $^{^{12}\}mathrm{The}$ derivation is intuitive. A more rigorous derivation can be found in Ryder chapter 6.4.

¹³A connected diagram is a diagram, where I can trace a path along the diagram between any two vertices.



Figure 1: E = 0 and V = 0



Figure 2: E = 0 and V = 2

- (iii) For each propagator we can rearrange the ends which results in a factor 2! for each propagator.
- (iv) Finally we can rearrange the propagators themselves and thus obtain another P! diagrams. These factors exactly cancel the factors in the double expansion. Thus we represent each vertex by a factor $ig \int d^4x$, a propagator by $\frac{1}{i}\Delta_F(x-x')$ and an external source by $i \int d^4x J(x)$.

This outlined counting of the diagrams generally leads to an overcounting for diagrams which possess a symmetry which corresponds to cases when a rearrangement of the functional derivatives can be exactly reverted by a change of the sources. For example for the first diagram in Fig. 2 we can swap the propagators which are connected to the same vertex and compensate it by swapping 2 derivatives yielding a factor 2^2 . Furthermore the propagator connecting the two vertices can be swapped and compensated for by swapping the two vertices. For the second diagram we can arrange the propagators in 3! ways and compensate this by exchanging the derivatives at each vertex. In addition, it is possible to simultaneously swap all propagators and compensate it by exchanging the vertices which yields another factor of 2. Thus the term corresponding to each diagram has to be divided by the symmetry factor S of the diagram.

The shown diagrams are all connected. In general there are also disconnected diagrams. A general diagram can be thought of as the product of the different connected subdiagrams and thus a general diagram

$$D = \frac{1}{S_D} \Pi_I C_I^{n_I} \tag{2.83}$$

where C_I denotes a connected diagram including its symmetry factor, n_I is the multiplicity for each connected diagram and S_D the symmetry factor from exchanging the different connected diagrams. As we already considered the symmetry factors of each individual connected diagram, the symmetry factor S_D can only account for rearrangements between diagrams. However we only end up with the same diagram, if we exchange all propagators and vertices of one diagram with an identical one and hence $S_D = \Pi_I n_I!$. The generating functional up to normalization is given by the sum over all diagrams

$$Z[J] \propto \sum D = \sum_{\{n_I\}} \prod_I \frac{1}{n_I!} C_I^{n_I} = \prod_I \sum_{n_I=0}^{\infty} \frac{1}{n_I!} C_I^{n_I} = \prod_I e^{C_I} = e^{\sum_I C_I} . \tag{2.84}$$

We find that the generating functional is given by the exponential of the sum of all connected diagrams. If we omit diagrams without any external sources in the sum, the so-called vacuum diagrams, we automatically obtain the correct normalization Z[0] = 1 and thus define the generating functional W for fully connected diagrams

$$iW[J] = \ln Z[J] = \sum_{I \neq \{0\}} C_I$$
 (2.85)

where the notation $I \neq \{0\}$ implies that vacuum diagrams are omitted.

We now calculate the vacuum expectation value of ϕ .

$$\langle 0|\phi(x)|0\rangle = \frac{1}{i} \frac{\delta}{\delta J(x)} Z[J] \bigg|_{J=0} = \frac{\delta}{\delta J(x)} W[J] \bigg|_{J=0} . \tag{2.86}$$

The leading order contribution at order $\mathcal{O}(g)$ can be obtained from the diagram on the right-hand side of Fig. 3, where the filled circle denotes a source. The source is removed by the derivative and thus we obtain

$$\langle 0|\phi(x)|0\rangle = \frac{1}{i}\frac{\delta}{\delta J(x)}\frac{1}{2}\left[ig\int d^4y\right]\left[i\int d^4y'J(y')\right]\frac{1}{i}\Delta_F(y-y')\frac{1}{i}\Delta_F(y-y) = -i\frac{g}{2}\Delta_F(0)\int d^4y\Delta_F(y-x)$$
(2.87)

with symmetry factor $\frac{1}{2}$. This is in contradiction with the requirement for the LSZ reduction formula which requires that $\langle 0|\phi(x)|0\rangle = 0$. Thus we have to modify our theory by introducing an additional term in the interaction Lagrangian, a so-called tadpole term, $Y\phi$

$$\mathcal{L}_1 = \frac{g}{6}\phi^3 + Y\phi \ . \tag{2.88}$$

It will lead to a new vertex which contributes a factor $iY \int d^4y$. In this modified theory there is a second contribution from the diagram on the left-hand side in Fig. 3 and thus

$$\langle 0|\phi(x)|0\rangle = \left(Y - i\frac{g}{2}\Delta_F(0)\right) \int d^4y \Delta_F(y-x) . \qquad (2.89)$$

By choosing Y we can ensure that the vacuum expectation value of the field vanishes as required by the LSZ reduction formula. This procedure is called renormalization. Let us evaluate $\Delta_F(0)$ to obtain the required value of Y

$$\Delta_F(0) = \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + m^2 - i\epsilon} \ . \tag{2.90}$$

This integral diverges quadratically! Thus we have to regularize the integral first before evaluating it. We are using cutoff regularization, where we impose a cutoff on the momentum in Euclidean space $|k_E| < \Lambda$. We first perform a so-called Wick rotation, $k^0 \to ik_E^4$, $k^i \to k_E^i$ to go from Minkowski space



Figure 3: Leading contribution to tadpole. Filled circle correspond to external source. x denotes vertex Y.

to Euclidean space, then use spherical coordinates to evaluate the integral.

$$i \int_{|k_E| < \Lambda} \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + m^2 - i\epsilon} = \int_{|k_E| < \Lambda} \frac{d^4k_E}{(2\pi)^4} \frac{1}{k_E^2 + m^2}$$
(2.91)

$$= \int d\Omega_4 \int_0^{\Lambda^2} \frac{k_E^2 dk_E^2}{2(2\pi)^4} \frac{1}{k_E^2 + m^2}$$
 (2.92)

$$= \frac{2\pi^2}{2(2\pi)^4} \int_{m^2}^{\Lambda^2 + m^2} dx \left(1 - \frac{m^2}{x}\right)$$
 (2.93)

$$= \frac{1}{16\pi^2} \left[x - m^2 \ln x \right]_{m^2}^{\Lambda^2 + m^2} \tag{2.94}$$

$$= \frac{1}{16\pi^2} \left[\Lambda^2 + m^2 \ln \left(1 + \frac{\Lambda^2}{m^2} \right) \right]$$
 (2.95)

where we used that the area of a d-dimensional unit sphere is given by

$$\int d\Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)} \tag{2.96}$$

and the substitution $x = k_E^2 + m^2$. Thus the leading divergence is quadratic and the second term diverges logarithmically. The tadpole coupling $Y = \frac{g}{2}i\Delta_F(0)$ is real as it is required for a hermitian Lagrangian.

Divergences in the evaluation of loop integrals are a common feature in quantum field theory. They are dealt with by first regularizing the integrals and then renormalizing couplings in the Lagrangian to absorb the divergences.

Summarising, the generating functional Z[J] can be expressed in terms of the generating functional W[J], which is given by the sum of all connected diagrams with no tadpoles and at least two sources J. The Lagrangian has to include all relevant couplings such that all divergences can be absorbed.

2.8 Scattering amplitudes and Feynman rules (10)

We are now in the position to calculate the probability for a transition from an initial state $|i\rangle$ to a final state $|f\rangle$. We consider the example of $2 \to 2$ scattering $1+2 \to 3+4$ and thus need the vacuum

expectation value of the time-ordered product of four field operators

$$\langle 0|T\phi(x_{1})\phi(x_{2})\phi(x_{3})\phi(x_{4})|0\rangle = \delta_{1}\delta_{2}\delta_{3}\delta_{4}Z[J]|_{J=0}$$

$$= \left[\delta_{1}\delta_{2}\delta_{3}\delta_{4}iW[J] + \delta_{1}\delta_{3}iW[J]\delta_{2}\delta_{4}iW[J] + \delta_{1}\delta_{4}iW[J]\delta_{2}\delta_{3}iW[J]\right]_{J=0}$$

$$= \langle 0|T\phi(x_{1})\phi(x_{2})\phi(x_{3})\phi(x_{4})|0\rangle_{C} - \Delta_{F}(x_{1} - x_{2})\Delta_{F}(x_{3} - x_{4})$$

$$- \Delta_{F}(x_{1} - x_{3})\Delta_{F}(x_{2} - x_{4}) - \Delta_{F}(x_{1} - x_{4})\Delta_{F}(x_{2} - x_{3})$$

$$(2.97)$$

$$+ \delta_{1}\delta_{2}iW[J]\delta_{3}\delta_{4}iW[J] + \delta_{1}\delta_{3}iW[J]\delta_{2}\delta_{4}iW[J] + \delta_{1}\delta_{4}iW[J]\delta_{2}\delta_{3}iW[J]\right]_{J=0}$$

$$= \langle 0|T\phi(x_{1})\phi(x_{2})\phi(x_{3})\phi(x_{4})|0\rangle_{C} - \Delta_{F}(x_{1} - x_{2})\Delta_{F}(x_{3} - x_{4})$$

$$- \Delta_{F}(x_{1} - x_{3})\Delta_{F}(x_{2} - x_{4}) - \Delta_{F}(x_{1} - x_{4})\Delta_{F}(x_{2} - x_{3})$$

$$(2.98)$$

where we used $Z[J] = \exp(iW[J])$, $\delta_i W[0] = 0$ and defined a short-hand for the functional derivative with respect to the source

$$\delta_i \equiv \frac{1}{i} \frac{\delta}{\delta J(x_i)} \ . \tag{2.100}$$

The first term corresponds to a fully connected diagram, where all four particles are connected to each other, while the others are products of 2-point functions and thus represent disconnected diagrams where always 2 particles are connected with a propagator. The LSZ reduction formula then determines the transition matrix element. Let us first consider how the disconnected diagrams contribute to the scattering amplitude. For example the contribution from $-\Delta_F(x_1 - x_3)\Delta_F(x_2 - x_4)$ can be separated

$$i^{4} \int e^{-ik_{1}x_{1} - ik_{2}x_{2} + ik_{3}x_{3} + ik_{4}x_{4}} \Pi_{i} d^{4}x_{i} (-\partial_{i}^{2} + m^{2}) \frac{1}{i} \Delta_{F}(x_{1} - x_{3}) \frac{1}{i} \Delta_{F}(x_{2} - x_{4}) = F_{13}F_{24}$$
 (2.101)

with

$$F_{13} = i \int d^4x_1 d^4x_3 \frac{d^4p}{(2\pi)^4} (p^2 + m^2) e^{-ik_1x_1 + ik_3x_3 + ip(x_1 - x_3)}$$
(2.102)

$$= i \int \frac{d^4p}{(2\pi)^4} (p^2 + m^2) (2\pi)^4 \delta(k_1 - p) (2\pi)^4 \delta(k_3 - p)$$
 (2.103)

$$= i(2\pi)^4 \delta(k_3 - k_1)(k_1^2 + m^2) \tag{2.104}$$

$$F_{24} = i(2\pi)^4 \delta(k_4 - k_2)(k_2^2 + m^2) . {(2.105)}$$

Thus the 4-momenta of the outgoing particles are equal to the ones of the incoming particles and it only contributes to forward scattering when the final state is the same as the initial state and thus does not contribute to the T matrix. The other two disconnected contributions are proportional to δ functions like $\delta(k_1 + k_2)$ with $k_1^0 + k_2^0 \ge 2m > 0$ and thus do not contribute. Generally only fully connected diagrams which are generated by taking derivatives of W are of interest.

Here the leading order is generated by the tree-level diagrams in Fig. 4. They translate to (We drop the subscript F from the Feynman propagator in the following.)

$$\delta_{1}\delta_{2}\delta_{3}\delta_{4}iW = (ig)^{2}\frac{1}{i^{5}}\int d^{4}xd^{4}y\Delta(x-y)\Big[\Delta(x_{1}-x)\Delta(x_{2}-x)\Delta(y-x_{3})\Delta(y-x_{4}) + \Delta(x_{1}-x)\Delta(x_{3}-x)\Delta(y-x_{2})\Delta(y-x_{4}) + \Delta(x_{1}-x)\Delta(x_{4}-x)\Delta(y-x_{2})\Delta(y-x_{3})\Big]$$

$$(2.106)$$

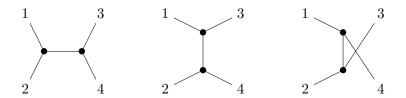


Figure 4: Tree-level diagrams contributing to $2 \rightarrow 2$ scattering

and thus it contributes to the S matrix as follows

$$ig^{2} \int d^{4}x d^{4}y e^{-ik_{1}x_{1} - ik_{2}x_{2} + ik_{3}x_{3} + ik_{4}x_{4}} \Pi_{i} d^{4}x_{i} \Delta(x - y) \Big[\delta(x_{1} - x)\delta(x_{2} - x)\delta(y - x_{3})\delta(y - x_{4}) + \delta(x_{1} - x)\delta(x_{3} - x)\delta(y - x_{2})\delta(y - x_{4}) + \delta(x_{1} - x)\delta(x_{4} - x)\delta(y - x_{2})\delta(y - x_{3}) \Big]$$

$$=ig^{2}\int d^{4}xd^{4}y\Delta(x-y)\left[e^{-i(k_{1}+k_{2})x+i(k_{3}+k_{4})y}+e^{-i(k_{1}-k_{3})x-i(k_{2}-k_{4})y}+e^{-i(k_{1}-k_{4})x-i(k_{2}-k_{3})y}\right]$$
(2.108)

$$=ig^{2}\int d^{4}xd^{4}y\frac{d^{4}p}{(2\pi)^{4}}\frac{e^{ip(x-y)}}{p^{2}+m^{2}-i\epsilon}\left[e^{-i(k_{1}+k_{2})x+i(k_{3}+k_{4})y}+e^{-i(k_{1}-k_{3})x-i(k_{2}-k_{4})y}+e^{-i(k_{1}-k_{4})x-i(k_{2}-k_{3})y}\right]$$
(2.109)

$$=ig^2\int d^4x d^4y \frac{d^4p}{(2\pi)^4} \frac{e^{-i(k_1+k_2-p)x+i(k_3+k_4-p)y} + e^{-i(k_1-k_3-p)x-i(k_2-k_4+p)y} + e^{-i(k_1-k_4-p)x-i(k_2-k_3+p)y}}{p^2+m^2-i\epsilon}$$

$$= i(2\pi)^4 g^2 \int d^4 p \frac{\delta(k_1 + k_2 - p)\delta(k_3 + k_4 - p) + \delta(k_1 - k_3 - p)\delta(k_2 - k_4 + p) + \delta(k_1 - k_4 - p)\delta(k_2 - k_3 + p)}{p^2 + m^2 - i\epsilon}$$
(2.111)

$$=-ig^{2}(2\pi)^{4}\delta(k_{1}+k_{2}-k_{3}-k_{4})\left[\frac{1}{s-m^{2}+i\epsilon}+\frac{1}{t-m^{2}+i\epsilon}+\frac{1}{u-m^{2}+i\epsilon}\right]$$
(2.112)

where we introduced the so-called Mandelstam variables

$$s = -(k_1 + k_2)^2 t = -(k_1 - k_3)^2 u = -(k_1 - k_4)^2 (2.113)$$

In the centre-of-mass frame s is simply given by the square of the total energy of the system $s = (E_1 + E_2)^2$. The Mandelstam variables satisfy

$$s + t + u = m_1^2 + m_2^2 + m_3^2 + m_4^2 . (2.114)$$

For general scattering processes it is convenient to define the matrix element M via

$$\langle f|i\rangle = iT_{fi} = i(2\pi)^4 \delta(k_{in} - k_{out})M \tag{2.115}$$

where k_{in} (k_{out}) is the sum of incoming (outgoing) momenta. Looking at our calculation we can derive a simple set of Feynman rules to calculate the matrix element:

- 1. Each external line corresponds to a factor 1.
- 2. For each internal line with momentum p write $\frac{i}{p^2-m^2+i\epsilon}$.
- 3. For each vertex write ig.
- 4. At each vertex the four-momentum is conserved.
- 5. Integrate over internal free momenta k_i with measure $d^4k_i/(2\pi)^4$.
- 6. Divide by symmetry factor of the diagram.
- 7. Sum over the expressions of the different diagrams.

Note momenta of incoming (outgoing) particles are going in (out).

3 Additional Material

3.1 Cross sections and Decay rates (11)

The probability for a transition from state $|i\rangle$ to state $|f\rangle$ is then given by

$$P = \frac{|\langle f|i\rangle|^2}{\langle f|f\rangle\langle i|i\rangle} \tag{3.1}$$

We will first consider a finite volume V and time interval T in order to avoid infinities and then take the continuum limit. Thus

$$(2\pi)^3 \delta^3(0) = \int d^3x e^{i0x} = V \qquad (2\pi)^4 \delta^4(0) = \int d^4x e^{i0x} = VT \qquad (3.2)$$

For definiteness we will consider the scattering of 2 particles to an arbitrary final state with n particles. The norm of a one-particle state is given by

$$\langle k|k\rangle = 2k^0(2\pi)^3\delta^3(0) = 2k^0V$$
 (3.3)

and as the two-particle state in the infinite past and future can be effectively described by the product of two one-particle states, we obtain

$$\langle i|i\rangle = 4E_1 E_2 V^2 \qquad \qquad \langle f|f\rangle = \Pi_i(2k_i^0 V) . \tag{3.4}$$

Similarly for the squared transition amplitude we obtain

$$|\langle f|i\rangle|^2 = |(2\pi)^4 \delta(k_{in} - k_{out})|^2 |M|^2 = (2\pi)^4 \delta(k_{in} - k_{out}) VT |M|^2.$$
(3.5)

Finally we have to sum over all possible final states. In the box with length L the 3-momenta are quantized $\vec{k}_i = \frac{2\pi}{L} \vec{n}_i$ and thus summing over the different modes corresponds to an integration

$$\sum_{n_i} \to \frac{L^3}{(2\pi)^3} \int d^3k_i \ . \tag{3.6}$$

The volume $V=L^3$ cancels against the volume factor from the normalization. Thus the transition rate is

$$\dot{P} = \frac{(2\pi)^4 \delta(k_{in} - k_{out})}{4E_1 E_2 V} \int \prod_{i=1}^n \frac{d^3 k_i}{(2\pi)^3 2\omega_i} |M|^2 . \tag{3.7}$$

The Lorentz-invariant differential cross section can be obtained by dividing by the incoming particle flux. In the rest frame of the second particle, it is simply given by the velocity of the first particle per volume. In the centre-of-mass frame (where the 3-momenta of the incoming particles add to zero), it is the relative velocity per volume $\sigma = \dot{P}V/v_{rel}$ where the relative velocity can be expressed by

$$v_{rel} = |\vec{v}_1 - \vec{v}_2| = \left| \frac{\vec{p}_1}{E_1} - \frac{\vec{p}_2}{E_2} \right| = \frac{|\vec{p}_1|}{E_1 E_2} (E_1 + E_2) = \frac{|\vec{p}_1|}{E_1 E_2} \sqrt{s}$$
(3.8)

In the last equation we introduced the so-called Mandelstam variable s. Scattering of 2 particles into 2 particles can be described in terms of 3 Lorentz-invariant quantities, the so-called Mandelstam variables

$$s = -(k_1 + k_2)^2 t = -(k_1 - k_3)^2 u = -(k_1 - k_4)^2 (3.9)$$

The differential cross section can also be written in terms of the flux factor 14

$$F = E_1 E_2 v_{rel} = \sqrt{s} \sqrt{E_1^2 - m_1^2} = \frac{1}{2} \sqrt{(s + m_1^2 - m_2^2)^2 - 4sm_1^2} = \sqrt{(p_1 \cdot p_2)^2 - m_1^2 m_2^2}$$
(3.11)

and thus expressed as

$$4Fd\sigma = |M|^2 dLIPS_n(k_1 + k_2). \tag{3.12}$$

The Lorentz-invariant n-body phase space is defined by

$$dLIPS_n(k) = (2\pi)^4 \delta\left(k - \sum_{i=1}^n k_i\right) \prod_{i=1}^n \frac{d^3 k_i}{(2\pi)^3 2\omega_i}.$$
 (3.13)

The 2-body phase space is particularly simple to evaluate in the centre-of-mass frame

$$\int d\text{LIPS}_2(k) = \int (2\pi)^4 \delta(k - k_1 - k_2) \frac{d^3 k_1}{(2\pi)^3 2\omega_1} \frac{d^3 k_2}{(2\pi)^3 2\omega_2}$$
(3.14)

$$= \int (2\pi)\delta(\sqrt{s} - E_1 - E_2) \frac{d^3k_1}{(2\pi)^3 2E_1 2E_2(k_1)}$$
(3.15)

$$= \int \delta(\sqrt{s} - E_1 - E_2) \frac{|\vec{k}_1| dE_1 d\Omega}{16\pi^2 E_2(E_1)} = \int \frac{d\Omega}{16\pi^2} \frac{|\vec{k}_1|}{\sqrt{s}}$$
(3.16)

$$= \int_{-1}^{1} \frac{d\cos\theta}{8\pi} \frac{|\vec{k}_1|}{\sqrt{s}} \tag{3.17}$$

where the last line holds if the integrand does not depend on the azimuthal angle ϕ .

In case that there are n identical particles in the final state, we have to divide by the symmetry factor S = n! in the cross section in order to avoid double-counting the different final state configurations. Thus the total cross section is given by

$$\sigma = \frac{1}{S} \int d\sigma \ . \tag{3.18}$$

If there is one particle in the initial state and we are studying decays we have to slightly modify our assumptions, because we assumed all particles to be stable in the previous discussion. However it turns out that the LSZ reduction formula also holds in this case. We only have to modify the initial state normalization $\langle i|i\rangle=2E_1V$ and find for the differential decay rate

$$d\Gamma = \frac{|M|^2}{2E_1} dLIPS_n(k_1)$$
(3.19)

$$E_1 = \frac{s + m_1^2 - m_2^2}{2\sqrt{s}} \tag{3.10}$$

which can be derived by using the definition of s and $\vec{p_1} + \vec{p_2} = 0$. For the last step in Eq. 3.11 we used $s = m_1^2 + m_2^2 - 2p_1 \cdot p_2$.

¹⁴The energy of one particle in the centre-of-mass frame is

and the total decay rate is obtained by summing over all outgoing momenta and dividing by the symmetry factor

$$\Gamma = \frac{1}{S} \int d\Gamma \ . \tag{3.20}$$

Note that the decay rate is not a Lorenz scalar. In the centre-of-mass frame of the particle, there is $E_1 = m_1$, while the decay rate is smaller in any other frame by a factor $\gamma = E_1/m_1$, the relativistic boost factor, which accounts for the relativistic time dilation. Faster particles have a longer lifetime, e.g. muons generated in the atmosphere reach the Earth's surface due to this time dilation factor.

3.2 Optical theorem

The S matrix is unitary because for two in-states $|i\rangle$ and $|j\rangle$ and the final (out-state) $|f\rangle$ we find

$$\sum_{f} S_{jf}^{*} S_{fi} = \sum_{f} \langle j|f\rangle \langle f|i\rangle = \langle j|i\rangle = \delta_{ij}$$
(3.21)

where we used the completeness of the out states $|f\rangle$. Thus the probability to scatter to any final state $|f\rangle$ is unity. It is often convenient to write the S matrix as

$$S = 1 + iT \tag{3.22}$$

where the identity refers to no scattering and the T matrix describes any (non-trivial) scattering. Then unitarity translates into

$$1 = S^{\dagger}S = (1 - iT^{\dagger})(1 + iT) = 1 + iT - iT^{\dagger} + T^{\dagger}T \qquad \Rightarrow \qquad T^{\dagger}T = -i(T - T^{\dagger}) = 2\text{Im}(T) \quad (3.23)$$

which is one form of the optical theorem.

3.3 Spin-statistics connection (4)

Could we quantize the scalar field also with anticommutators instead of commutators? Consider spin-0 particles with the Hamiltonian

$$H_0 = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \omega_k a^{\dagger}(k) a(k). \tag{3.24}$$

The creation and annihilation operators either satisfy commutation or anticommutation relations

$$[a(k), a(k')]_{\mp} = [a^{\dagger}(k), a^{\dagger}(k')]_{\mp} = 0 \qquad [a(k), a^{\dagger}(k')]_{\mp} = (2\pi)^3 2\omega_k \delta^3(k - k')$$
 (3.25)

Now construct a theory with local Lorentz-invariant interactions out of the non-hermitian fields

$$\phi^{+}(x,0) = \int \frac{d^{3}k}{(2\pi)^{3}2\omega_{k}} e^{i\vec{k}\cdot\vec{x}}a(k) \qquad \qquad \phi^{-}(x,0) = \int \frac{d^{3}k}{(2\pi)^{3}2\omega_{k}} e^{-i\vec{k}\cdot\vec{x}}a^{\dagger}(k)$$
(3.26)

$$\phi^{\pm}(x,t) = e^{iH_0t}\phi^{\pm}(x,0)e^{-iH_0t} = \int \frac{d^3k}{(2\pi)^3 2\omega_k} e^{\pm ikx} a^{(\dagger)}(k)$$
 (3.27)

which are related by hermitian conjugation $\phi^+ = (\phi^-)^{\dagger}$. $\phi^{\pm}(x,t)$ is the time-evolved field $\phi^{\pm}(x,0)$. The field ϕ is invariant under proper orthochronous Lorentz transformations Λ

$$U(\Lambda)^{-1}\phi(x)U(\Lambda) = \phi(\Lambda^{-1}x)$$
(3.28)

and thus also the creation $(a^{\dagger}(k))$ and annihilation (a(k)) operators as well as the fields $\phi^{\pm}(x)$ are Lorentz scalars. Construct an interaction Lagrangian density \mathcal{L}_1 which is local and Lorentz invariant. The corresponding Hamiltonian density is denoted by \mathcal{H}_1 and H_1 denotes the interaction Hamiltonian in the Schrödinger picture

$$H_1 = \int d^3x \mathcal{H}_1(x,0)$$
 (3.29)

where $\mathcal{H}_1(x,0)$ is a hermitian function of $\phi^{\pm}(x,0)$. The corresponding Hamiltonian density in the interaction picture $\mathcal{H}_I(x,t)$ is defined by the same function, but with $\phi^{\pm}(x,0)$ replaced by $\phi^{\pm}(x,t)$, since the interaction Hamiltonian is given by $H_I(t) = \exp(-iH_0t)H_1 \exp(iH_0t)$.

Consider now a transition amplitude from a state $|i\rangle$ at $t=-\infty$ to state $|f\rangle$ at $t=\infty$

$$\mathcal{T}_{f \leftarrow i} = \left\langle f | T \exp\left[-i \int_{-\infty}^{\infty} dt H_I(t)\right] | i \right\rangle . \tag{3.30}$$

The transition amplitude is only Lorentz invariant, if the time-ordering is frame independent. This is trivially satisfied in the forward and backward lightcone for time-like separations of two events $(x - x')^2 > 0$. However events with a space-like separation can have different temporal ordering. Thus we have to require that the interaction Hamiltonian commutes with itself at different times for space-like separations

$$[\mathcal{H}_I(x), \mathcal{H}_I(x')] = 0 \qquad (x - x')^2 > 0 \tag{3.31}$$

The interaction Hamiltonian densities are constructed of the fields $\phi^{\pm}(x,t)$ and thus we have to consider the commutator (anticommutator) of the fields ϕ^{\pm} for space-like separations $r^2 \equiv (x-x')^2 > 0$

$$[\phi^{+}(x), \phi^{-}(x')]_{\mp} = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \frac{d^3k'}{(2\pi)^3 2\omega_k'} e^{i(kx-k'x')} [a(k), a^{\dagger}(k')]_{\mp} = \int \frac{d^3k}{(2\pi)^3 2\omega_k} e^{ik(x-x')}$$
(3.32)

The integral is best evaluated for t=t' using spherical coordinates. For $t=t',\,k=|\vec{k}|$ and $r=|\vec{x}-\vec{x}'|$

$$\frac{1}{8\pi^2} \int_0^\infty dk \int_{-1}^1 d\cos\theta \frac{k^2}{E(k)} e^{ikr\cos\theta} = \frac{1}{8\pi^2} \int_0^\infty dk \frac{k^2}{E(k)} \frac{e^{ikr} - e^{-ikr}}{ikr} = -\frac{i}{8\pi^2 r} \int_{-\infty}^\infty dk \frac{k}{\sqrt{k^2 + m^2}} e^{ikr} . \tag{3.33}$$

The integrand has branch cuts along the imaginary axis starting at $\pm im$. We deform the integration contour such that it wraps around the upper branch cut by defining $\rho = ik/m$ and thus

$$[\phi^{+}(x), \phi^{-}(x')]_{\mp} = \frac{m}{4\pi^{2}r} \int_{1}^{\infty} d\rho \frac{\rho e^{-\rho mr}}{\sqrt{\rho^{2} - 1}} = \frac{m}{4\pi^{2}r} \int_{1}^{\infty} d\rho \left(\frac{\partial}{\partial \rho} \sqrt{\rho^{2} - 1}\right) e^{-\rho mr}$$
(3.34)

$$= \frac{m}{4\pi^2 r} \left\{ \left[\sqrt{\rho^2 - 1} e^{-\rho mr} \right]_1^{\infty} - \int_1^{\infty} d\rho \sqrt{\rho^2 - 1} \frac{\partial}{\partial \rho} e^{-\rho mr} \right\}$$
(3.35)

$$= \frac{m^2}{4\pi^2} \int_1^\infty d\rho \sqrt{\rho^2 - 1} e^{-\rho mr} = \frac{m}{4\pi^2 r} K_1(mr) \equiv C(r)$$
 (3.36)

where K_1 denotes the modified Bessel function. Thus the (anti)commutator is non-zero for any r > 0. Consider now the linear combination $\phi_{\lambda}(x) = \phi^{+}(x) + \lambda \phi^{-}(x)$ with an arbitrary complex number λ . The (anti)commutators of ϕ_{λ} for space-like separations are then

$$[\phi_{\lambda}(x), \phi_{\lambda}^{\dagger}(x')]_{\mp} = [\phi^{+}(x), \phi^{-}(x')]_{\mp} + |\lambda|^{2} [\phi^{-}(x), \phi^{+}(x')]_{\mp} = (1 - |\lambda|^{2}) C(r)$$
(3.37)

$$[\phi_{\lambda}(x), \phi_{\lambda}(x')]_{\mp} = \lambda[\phi^{+}(x), \phi^{-}(x')]_{\mp} + \lambda[\phi^{-}(x), \phi^{+}(x')]_{\mp} = \lambda(1 \mp 1)C(r)$$
(3.38)

Thus in order for both (anti)commutators to vanish and to have a suitable interaction Hamiltonian built out of the field ϕ_{λ} we have to choose commutators with $|\lambda| = 1$. This brings us back to a real scalar field if we choose $\lambda = e^{i\alpha}$, then $e^{-i\alpha/2}\phi_{\lambda}(x) = \phi(x)$.

The same argument can be made for higher spin fields in any number of space-time dimensions¹⁵. The allowed choice is always commutators for integer spin and anticommutators for half-integer spin. Hence particles with integer spin are bosons and particles with half-integer spin fermions.

3.4 Complex scalar field (22)

So far we considered a real scalar field. For a complex scalar field the discussion is very similar, but there are a few important differences. The Lagrangian of a free complex scalar field ϕ is given by

$$\mathcal{L} = -\partial_{\mu}\phi^{\dagger}\partial^{\mu}\phi - m^{2}\phi^{\dagger}\phi \tag{3.39}$$

The Lagrangian is invariant under an internal symmetry $\phi \to e^{-iq\alpha}\phi$, where q is the charge of the field, and thus there is a Noether current and we obtain

$$J_{\mu} = -iq \left[(\partial_{\mu} \phi^{\dagger}) \phi - (\partial_{\mu} \phi) \phi^{\dagger} \right] = iq \phi^{\dagger} \stackrel{\leftrightarrow}{\partial_{\mu}} \phi$$
 (3.40)

and a conserved charge

$$Q = iq \int d^3x \phi^{\dagger} \stackrel{\leftrightarrow}{\partial_t} \phi . \tag{3.41}$$

The Euler-Lagrange equations and conjugate momenta are

$$(\Box - m^2)\phi = 0 \qquad (\Box - m^2)\phi^{\dagger} = 0 \qquad (3.42)$$

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi}^{\dagger} \qquad \qquad \pi^{\dagger} = \frac{\partial \mathcal{L}}{\partial \dot{\phi}^{\dagger}} = \dot{\phi} \qquad (3.43)$$

The general solution for the fields ϕ and ϕ^{\dagger} are given by

$$\phi(x,t) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left(a(k)e^{ikx} + b^{\dagger}(k)e^{-ikx} \right)$$
 (3.44)

$$\phi^{\dagger}(x,t) = \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left(a^{\dagger}(k)e^{-ikx} + b(k)e^{ikx} \right) . \tag{3.45}$$

¹⁵For d=2 there are more possibilities apart from fermions and bosons, so-called anyons.

We quantize it in the usual way, but we have to keep in mind that ϕ and ϕ^{\dagger} are independent. The equal time commutation relations are

$$[\pi(x,t),\phi(y,t)] = [\pi^{\dagger}(x,t),\phi^{\dagger}(y,t)] = -i\delta^{3}(x-y)$$
(3.46)

while all other equal time commutation relations vanish. This leads to the following commutation relations for the operators a(k) and b(k)

$$[a(k), a^{\dagger}(k')] = [b(k), b^{\dagger}(k')] = (2\pi)^3 2\omega_k \delta(\vec{k} - \vec{k}')$$
(3.47)

where a(k) and b(k) are annihilation operators. Thus there are two types of particles, a and b, with Hamiltonian

$$H = \int d\frac{d^3k}{(2\pi)^3 2\omega_k} \omega_k \left[a^{\dagger}(k)a(k) + b^{\dagger}(k)b(k) \right] . \tag{3.48}$$

Thus the particles both have the same positive energy, but they have equal and opposite charges, because the charge operator is given by

$$Q = q \int \int \frac{d^3k}{(2\pi)^3 2\omega_k} \left[a^{\dagger}(k)a(k) - b^{\dagger}(k)b(k) \right] . \tag{3.49}$$

Otherwise their properties including mass are equivalent. They form a pair of particle and antiparticle. The existence of antiparticles is a general feature of relativistic quantum field theory.

3.5 Free scalar field - ground state wave function (Weinberg)

In this section, we how the $i\epsilon$ factor enters the Lagrangian. The Lagrangian density of a free real scalar field is given by

$$\mathcal{L} = -\frac{1}{2}\partial_{\mu}\phi\partial^{\mu}\phi - \frac{m^2}{2}\phi^2 \tag{3.50}$$

and the conjugate momentum $\pi = \dot{\phi}$. The relevant equal-time commutation relations are

$$[\pi(x,t),\phi(y,t)] = -i\delta(x-y) \qquad [\pi(x,t),\pi(y,t)] = [\phi(x,t),\phi(y,t)] = 0 \qquad (3.51)$$

and the annihilation operator is defined as

$$a(k) = \int d^3x e^{-ikx} \left[i\pi(x) + \omega_k \phi(x) \right] .$$
 (3.52)

We follow the discussion of the quantum harmonic oscillator to obtain the ground state for a given time t. In the field ϕ basis, the conjugate momentum is given by $\pi(x,t) = -i\frac{\delta}{\delta\phi(x,t)}$ and thus the defining equation of the ground state is

$$0 = \int d^3x e^{-ikx} \left[\frac{\delta}{\delta \phi(x,t)} + \omega_k \phi(x,t) \right] \langle \phi; t | 0 \rangle$$
 (3.53)

In analogy to the quantum harmonic oscillator we use a Gaussian ansatz for the ground state wave function

$$\langle \phi; t | 0 \rangle = N \exp\left(-\frac{1}{2} \int d^3x d^3y \mathcal{E}(x, y) \phi(x, t) \phi(y, t)\right) .$$
 (3.54)

It provides a solution provided that

$$0 = \int d^3x e^{i\omega_k t} e^{-i\vec{k}\cdot\vec{x}} \left[-\int d^3y \mathcal{E}(x,y)\phi(y,t) + \omega_k \phi(x,t) \right]$$
(3.55)

is satisfied for all ϕ . We can rewrite it as follows

$$0 = \int d^3x e^{i\omega_k t} e^{-i\vec{k}\cdot\vec{x}} \left[-\int d^3y \mathcal{E}(x,y)\phi(y,t) + \int d^3y \delta(x-y)\omega_k \phi(y,t) \right]$$
(3.56)

$$= \int d^3y \left[-\int d^3x e^{-i\vec{k}\cdot\vec{x}} \mathcal{E}(x,y) + e^{-i\vec{k}\cdot\vec{y}} \omega_k \right] \phi(y,t) e^{i\omega_k t} . \tag{3.57}$$

As the equation holds for all ϕ and the expression in the square brackets is a smooth function, the expression in the square brackets has to vanish identically. Inverting the Fourier transform we find for the kernel

$$\mathcal{E}(x,y) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{x}-\vec{y})} \sqrt{\vec{k}^2 + m^2} \ . \tag{3.58}$$

This also holds in the infinite past and future (even for an interacting real scalar field theory) and thus

$$\langle 0; \operatorname{out} | \phi(x, \infty); \infty \rangle \langle \phi(x, -\infty); -\infty | 0; \operatorname{in} \rangle \tag{3.59}$$

$$=|N|^2 \exp\left(-\frac{1}{2} \int d^3x d^3y \mathcal{E}(x,y) \left[\phi(x,\infty)\phi(y,\infty) + \phi(x,-\infty)\phi(y,-\infty)\right]\right) (3.60)$$

$$= \lim_{\epsilon \to 0^+} |N|^2 \exp\left(-\frac{\epsilon}{2} \int d^3x d^3y \int_{-\infty}^{\infty} d\tau \mathcal{E}(x, y) \phi(x, \tau) \phi(y, \tau) e^{-\epsilon|\tau|}\right)$$
(3.61)

This term will slightly shift the poles in the complex E plane and thus will determine the form of the Green's function like in the case of the quantum harmonic oscillator. The generating functional in this case is given by

$$Z[J] = \frac{\int \mathcal{D}\phi \exp\left(i \int d^4x \left(\mathcal{L} + J(x)\phi(x)\right) - \frac{\epsilon}{2} \int d^3x d^3y d\tau \mathcal{E}(x,y)\phi(x,\tau)\phi(y,\tau)\right)}{\int \mathcal{D}\phi \exp\left(i \int d^4x \mathcal{L} - \frac{\epsilon}{2} \int d^3x d^3y d\tau \mathcal{E}(x,y)\phi(x,\tau)\phi(y,\tau)\right)}$$
(3.62)

$$= \frac{\int \mathcal{D}\phi \exp\left(-\frac{i}{2} \int d^4x d^4x' \phi(x) \phi(x') D(x, x') + i \int d^4x J(x) \phi(x)\right)}{\int \mathcal{D}\phi \exp\left(-\frac{i}{2} \int d^4x d^4x' \phi(x) \phi(x') D(x, x')\right)}$$
(3.63)

where we dropped the factor $e^{-\epsilon|\tau|}$ in the first line and it is understood that in the end the limit $\epsilon \to 0$ is taken. D(x,y) in the second line is defined as

$$D(x,x') = \frac{\partial}{\partial x'_{\mu}} \frac{\partial}{\partial x^{\mu}} \delta(x-x') + m^2 \delta(x-x') - i\epsilon \mathcal{E}(\vec{x}, \vec{x}') \delta(t-t') . \tag{3.64}$$

All three terms only depend on the difference x - x' and thus the result is translation invariant. In momentum space with

$$\tilde{\phi}(p) = \int d^4x e^{-ipx} \phi(x) \qquad \qquad \phi(x) = \int \frac{d^4p}{(2\pi)^4} e^{ipx} \tilde{\phi}(p)$$
 (3.65)

we thus obtain

$$\tilde{D}(p) = p^2 + m^2 - i\epsilon E(p) \tag{3.66}$$

$$S + J\phi + i\epsilon \text{ terms} = \frac{1}{2} \int \frac{d^4p}{(2\pi)^4} \left(-\tilde{\phi}(p)\tilde{D}(p)\tilde{\phi}(-p) + \tilde{J}(p)\tilde{\phi}(-p) + \tilde{J}(-p)\tilde{\phi}(p) \right)$$
(3.67)

As we are only interested in the limit $\epsilon \to 0^+$, it is common to replace $i\epsilon E(p)$ by $i\epsilon$ which we will do in the following for simplicity. Thus the expressions $\tilde{D}(p)$ and D(x, x') reduce to

$$\tilde{D}(p) = p^2 + m^2 - i\epsilon \tag{3.68}$$

$$D(x,x') = \left[\frac{\partial}{\partial x'_{\mu}} \frac{\partial}{\partial x^{\mu}} + m^2 - i\epsilon\right] \delta(x - x') . \tag{3.69}$$

A Review

A.1 Quantum harmonic oscillator

The last 1D example which we are studying is the harmonic oscillator. It is very important approximation to many physical phenomena such as the vibrational modes of a diatomic molecule as shown in Fig. 5. A particle with mass m is subject to a restoring force -kx, where x is the displacement

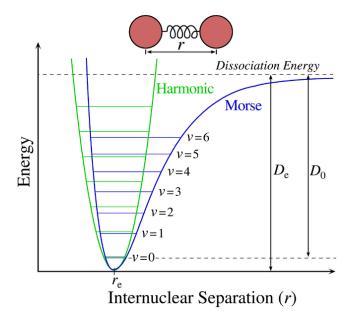


Figure 5: First few vibrational modes of a diatomic molecule are well described by a harmonic oscillator. Figure taken from https://en.wikipedia.org/wiki/File:Morse-potential.png.

from the equilibrium position. The potential energy of the particle is

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$$
 (A.1)

where $\omega = \sqrt{k/m}$ is the angular oscillation frequency. Thus its Hamiltonian is

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \tag{A.2}$$

and the time-independent Schrödinger equation is given by

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\varphi_E(x) = E\varphi_E(x) . \tag{A.3}$$

Now we will be going one step and solve the quantum harmonic oscillator using the ladder operator method.

In order to simplify our following discussion, we define the variable

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x \qquad \frac{d}{d\xi} = \sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx}$$
 (A.4)

and can rewrite our Hamiltonian in Eq. (A.2) as follows

$$H = \frac{1}{2}\hbar\omega \left(-\frac{d^2}{d\xi^2} + \xi^2 \right) \tag{A.5}$$

In the next step we want to factorise the Hamiltonian in analogy to the identity

$$u^{2} - v^{2} = (u - v)(u + v). (A.6)$$

Hence we form two new operators as linear combination of the old ones

$$a = \frac{1}{\sqrt{2}} \left(\xi + \frac{d}{d\xi} \right) = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + i \frac{\hat{p}}{m\omega} \right) \tag{A.7}$$

$$a^{\dagger} = \frac{1}{\sqrt{2}} \left(\xi - \frac{d}{d\xi} \right) = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - i \frac{\hat{p}}{m\omega} \right) .$$
 (A.8)

The operators satisfy the following commutation relation

$$[a, a^{\dagger}] = 1. \tag{A.9}$$

Looking at the product of the two operators

$$a^{\dagger}a = \frac{1}{\sqrt{2}} \left(\xi - \frac{d}{d\xi} \right) \frac{1}{\sqrt{2}} \left(\xi + \frac{d}{d\xi} \right) \tag{A.10}$$

$$= \frac{1}{2} \left(\xi^2 - \frac{d^2}{d\xi^2} + \xi \frac{d}{d\xi} - \frac{d}{d\xi} \xi \right)$$
 (A.11)

$$=\frac{1}{2}\left(\xi^2 - \frac{d^2}{d\xi^2} + \left[\xi, \frac{d}{d\xi}\right]\right) \tag{A.12}$$

$$= \frac{1}{2} \left(\xi^2 - \frac{d^2}{d\xi^2} - 1 \right) \tag{A.13}$$

we observe that we almost obtain the result which we wanted to obtain. Hence, the Hamiltonian can be rewritten as

$$H = \hbar\omega \left(a^{\dagger} a + \frac{1}{2} \right) . \tag{A.14}$$

Before interpreting the operators \hat{a} and \hat{a}^{\dagger} physically, we have to show two more commutation relations:

$$[H, a] = Ha - aH \tag{A.15}$$

$$= \hbar\omega \left(a^{\dagger} a + \frac{1}{2} \right) a - a\hbar\omega \left(a^{\dagger} a + \frac{1}{2} \right) \tag{A.16}$$

$$= \hbar\omega \left(a^{\dagger}aa - aa^{\dagger}a \right) \tag{A.17}$$

$$= \hbar\omega \left(a^{\dagger}aa - \left(a^{\dagger}a + [a, a^{\dagger}] \right) a \right) \tag{A.18}$$

$$= -\hbar\omega a \tag{A.19}$$

Now given an energy eigenstate $|E\rangle$ with a given energy E, we can calculate the energy eigenvalue of the states $a|E\rangle$ as follows

$$H(a|E\rangle) = Ha|E\rangle \tag{A.20}$$

$$= (aH + [H, a]) |E\rangle \tag{A.21}$$

$$= (aE - \hbar\omega a) |E\rangle \tag{A.22}$$

$$= (E - \hbar\omega)(a|E\rangle) \tag{A.23}$$

Similarly for the operator a^{\dagger}

$$[H, a^{\dagger}] = +\hbar\omega a^{\dagger} . \tag{A.24}$$

and

$$H(a^{\dagger} | E \rangle) = (E + \hbar \omega)(a^{\dagger} | E \rangle) . \tag{A.25}$$

Hence the states $a|E\rangle$, $a^{\dagger}|E\rangle$ are also energy eigenstates with energies $E \pm \hbar\omega$, respectively. The operators a and a^{\dagger} transform a state with energy E into a state with energy $E \pm \hbar\omega$. They are denoted ladder operators, more specifically a^{\dagger} is denoted raising operator and a lowering operator.

Next we have to find the lowest energy eigenstate or ground state. Classically we observe that there is a minimum energy of the harmonic oscillator. Hence there has to be a lowest energy eigenstate

$$a | E_{lowest} \rangle = 0$$
. (A.26)

This is called the *ladder termination condition*. The energy of this lowest energy eigenstate is given by

$$H|E_{lowest}\rangle = \hbar\omega \left(a^{\dagger}a + \frac{1}{2}\right)|E_{lowest}\rangle = \frac{1}{2}\hbar\omega |E_{lowest}\rangle .$$
 (A.27)

Note that lowest energy level is not zero as it would be for a classical harmonic oscillator, but $\frac{1}{2}\hbar\omega$. It is known as zero point energy and ultimately due to the non-vanishing commutator of the ladder operators $[a, a^{\dagger}] = 1$. The lowest energy eigenstate is commonly denoted $|0\rangle$. The energy of the n^{th} state $|n\rangle$ is given by

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right) , \qquad (A.28)$$

because applying the raising operator a^{\dagger} n times increases the energy with respect to the lowest energy eigenstate by $n \times \hbar \omega$. In addition to the ladder operators it is convenient to introduce the *number operator*,

$$\hat{N} = \hat{a}^{\dagger} \hat{a} , \qquad (A.29)$$

which counts the energy quanta. It fulfils the following eigenvalue equation

$$\hat{N} |n\rangle = n |n\rangle , \qquad (A.30)$$

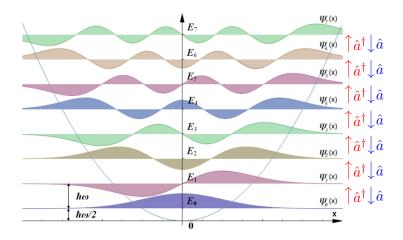


Figure 6: Energy levels of harmonic oscillator. Raising operator a^{\dagger} increases energy by $\hbar\omega$ and lowering operator a lowers it. Figure taken from https://commons.wikimedia.org/w/index.php?curid=11623546.

where the n in $|n\rangle$ denotes the number of energy quanta. We can rewrite the Hamiltonian as

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2}\right) . \tag{A.31}$$

See Fig. 6 for an illustration of the action of the ladder operator on the energy eigenstates. All other energy eigenstates can be constructed from the lowest energy eigenstate using the raising operator. By demanding that all states $|n\rangle$ are properly normalised,

$$\langle n|n\rangle = 1 \,, \tag{A.32}$$

it is possible to show 16 that the raising and lowering operators act on a state $|n\rangle$

$$a|n\rangle = \sqrt{n}|n-1\rangle \tag{A.33}$$

$$a^{\dagger} | n \rangle = \sqrt{n+1} | n+1 \rangle$$
 (A.34)

Thus we can write the state $|n\rangle$ as follows

$$|n\rangle \equiv \frac{1}{\sqrt{n!}} \left(a^{\dagger} \right)^n |0\rangle , \qquad (A.35)$$

where we denoted the lowest energy eigenstate by $|0\rangle$. The factor $1/\sqrt{n!}$ ensures that the states are correctly normalised.

The wave function of the lowest energy eigenstate $\phi_0(\xi)$ can be determined from the ladder termination condition in Eq. (A.26)

$$0 = a\phi_0(\xi) = \frac{1}{\sqrt{2}} \left(\xi + \frac{d}{d\xi} \right) \phi_0(\xi) . \tag{A.36}$$

¹⁶See the discussion in McIntyre Chap.9.

It is an ODE, which can be solved using standard techniques

$$\phi_0(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2} \ . \tag{A.37}$$

The explicit form of the wave function involves a well studied special function, the Hermite polynomial, such that the normalised wave functions can be written as

$$\varphi_E(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \quad \text{with } \xi = \sqrt{\frac{m\omega}{\hbar}} x \text{ and } n = 0, 1, 2, 3, \dots$$
 (A.38)

where H_n is a Hermite polynomial of order n

$$H_0(x) = 1,$$
 $H_1(x) = 2x,$ $H_2(x) = 4x^2 - 2$ $H_3(x) = 8x^3 - 12x$. (A.39)

Figure 7 shows wave functions and probability densities for the first four energy levels of a harmonic oscillator.

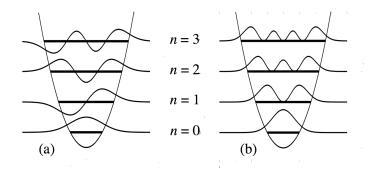


Figure 7: (a) Wave functions and (b) the probability density for the first four energy levels of a harmonic oscillator.

A.2 Time-dependent perturbation theory in quantum mechanics

As we are dealing with a time-dependent Hamiltonian, we have to return to the Schrödinger equation in its original form. So far we always considered the Hamiltonian to be time-independent, while the quantum states evolved with time. This is commonly denoted as *Schrödinger picture*. If we however consider the states¹⁷

$$|\psi\rangle_{H} \equiv e^{i\hat{H}t/\hbar} |\psi(t)\rangle = \left(1 + \frac{i}{\hbar}\hat{H}t + \frac{1}{2} \left[\frac{i}{\hbar}\hat{H}t\right]^{2}\right) |\psi(t)\rangle \tag{A.40}$$

we find that

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle_{H} = i\hbar\frac{\partial}{\partial t}e^{i\hat{H}t/\hbar}\left|\psi(t)\right\rangle = e^{i\hat{H}t/\hbar}\left(-\hat{H}\left|\psi(t)\right\rangle + i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle\right) = 0 \tag{A.41}$$

¹⁷Note that $e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{1}{n!} \hat{A}^n$.

This is commonly denoted as *Heisenberg picture*. In this picture, all operators

$$\hat{A}_H(t) = e^{i\hat{H}t/\hbar} \hat{A}e^{-i\hat{H}t/\hbar} , \qquad (A.42)$$

e.g. momentum operator, will be time-dependent and satisfy

$$\frac{d}{dt}\hat{A}_H(t) = \frac{i}{\hbar}[\hat{H}_H(t), \hat{A}_H(t)] + \left(\frac{\partial \hat{A}}{\partial t}\right)_H. \tag{A.43}$$

Thus the eigenvalues of any operator, which commutes with the Hamiltonian, are contants and provide good quantum numbers to describe the system. We will now consider the *interaction picture*, in which both the Hamiltonian and the quantum state will depend on time. It is useful for cases, where we can split the Hamiltonian $\hat{H}(t) = \hat{H}_0 + \hat{H}'(t)$ in a time-independent part \hat{H}_0 and a time-dependent one \hat{H}' . It is defined by

$$|\psi(t)\rangle_I = e^{i\hat{H}_0 t/\hbar} |\psi(t)\rangle$$
 $\hat{A}_I(t) = e^{i\hat{H}_0 t/\hbar} \hat{A} e^{-i\hat{H}_0 t/\hbar}$. (A.44)

We rewrite the Schrödinger equation for the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}'(t)$ in the interaction picture

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = i\hbar \frac{\partial}{\partial t} e^{i\hat{H}_0 t/\hbar} |\psi(t)\rangle \tag{A.45}$$

$$= -\hat{H}_0 |\psi(t)\rangle_I + e^{i\hat{H}_0 t/\hbar} i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \tag{A.46}$$

$$= -\hat{H}_0 |\psi(t)\rangle_I + e^{i\hat{H}_0 t/\hbar} \left(\hat{H}_0 + \hat{H}'(t)\right) |\psi(t)\rangle \tag{A.47}$$

$$= -\hat{H}_0 |\psi(t)\rangle_I + e^{i\hat{H}_0 t/\hbar} \left(\hat{H}_0 + \hat{H}'(t)\right) e^{-i\hat{H}_0 t/\hbar} |\psi(t)\rangle_I$$
 (A.48)

$$=e^{i\hat{H}_0t/\hbar}\hat{H}'(t)e^{-i\hat{H}_0t/\hbar}|\psi(t)\rangle_I \tag{A.49}$$

$$=\hat{H}_{I}'(t)|\psi(t)\rangle_{I}. \tag{A.50}$$

We used that the exponential $\exp(iH_0t/\hbar)$ commutes with H_0 . Finally, we can now formally integrate the equation and obtain the equivalent integral equation

$$|\psi(t)\rangle_I = |\psi(t_0)\rangle_I + \frac{1}{i\hbar} \int_{t_0}^t \hat{H}_I'(t') \left|\psi(t')\rangle_I dt'.$$
 (A.51)

This integral equation can be iteratively solved by plugging the solution back in on the right-hand side of the equation, i.e.

$$|\psi(t)\rangle_{I} = |\psi(t_{0})\rangle_{I} + \frac{1}{i\hbar} \int_{t_{0}}^{t} \hat{H}'_{I}(t') |\psi(t_{0})\rangle_{I} dt' + \left(\frac{1}{i\hbar}\right)^{2} \int_{t_{0}}^{t} dt' \int_{t_{0}}^{t'} dt'' \hat{H}'_{I}(t') \hat{H}'_{I}(t'') |\psi(t_{0})\rangle_{I} + \dots$$
(A.52)

We introduce the time-ordered product of operators to simplify the expression further. The time-ordered product of two operators A and B is defined as

$$\mathcal{T}(A(t_1)B(t_2)) \equiv \begin{cases} A(t_1)B(t_2) & \text{for } t_1 \ge t_2 \\ B(t_2)A(t_1) & \text{otherwise} \end{cases}$$
 (A.53)

This allows us to rewrite the quadratic term as

$$\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{H}_I'(t') \hat{H}_I'(t'') = \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \mathcal{T} \left(\hat{H}_I'(t') \hat{H}_I'(t'') \right) = \mathcal{T} \left(\int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \hat{H}_I'(t') \hat{H}_I'(t'') \right)$$

$$= \mathcal{T} \left(\int_{t_0}^t dt'' \int_{t_0}^{t''} dt' \hat{H}_I'(t'') \hat{H}_I'(t'') \right) = \mathcal{T} \left(\int_{t_0}^t dt'' \int_{t_0}^{t''} dt' \hat{H}_I'(t') \hat{H}_I'(t'') \right)$$

$$= \frac{1}{2} \mathcal{T} \left(\int_{t_0}^t dt' \int_{t_0}^t dt'' \hat{H}_I'(t') \hat{H}_I'(t'') \right) = \frac{1}{2} \mathcal{T} \left(\int_{t_0}^t dt' \hat{H}_I'(t') \right)^2 , \quad (A.56)$$

where we introduced the time-ordered product in the first line, relabelled the integration variables $t' \leftrightarrow t''$ in the second line, and noticed that summing the last terms of the first and second line and dividing by 2 can be rewritten as the first term of the third line. Hence we can write the quadratic term as the square of the integral and

$$|\psi(t)\rangle_{I} = |\psi(t_{0})\rangle_{I} + \frac{1}{i\hbar} \int_{t_{0}}^{t} \hat{H}'_{I}(t')dt' |\psi(t_{0})\rangle_{I} + \frac{1}{2}\mathcal{T} \left(\frac{1}{i\hbar} \int_{t_{0}}^{t} dt' H'_{I}(t')\right)^{2} |\psi(t_{0})\rangle_{I} + \dots$$

$$= \mathcal{T} \left(e^{-\frac{i}{\hbar} \int_{t_{0}}^{t} \hat{H}'_{I}(t')dt'}\right) |\psi(t_{o})\rangle_{I} .$$
(A.57)

We will only consider the leading order transitions and neglect terms with more than one \hat{H}' . If we have the set of eigenstates $|n\rangle$ to the Hamiltonian \hat{H}_0 with eigenvalue E_n , we can calculate the transition amplitude to find our particle in state $|n\rangle$ at time t if we start in state $|m\rangle$ at time t_0 . The system is initially in the state

$$|m(t)\rangle = e^{-iH_0t/\hbar} |m\rangle = e^{-iE_mt/\hbar} |m\rangle ,$$
 (A.59)

where $|m(t)\rangle$ denotes the state $|m\rangle$ which has been evolved to time t with the Hamiltonian H_0 . The probability amplitude that there is a transition to the state

$$|n(t)\rangle = e^{-iH_0t/\hbar} |n\rangle = e^{-iE_nt/\hbar} |n\rangle$$
 (A.60)

is given by

$$\langle n(t)|\psi(t)\rangle = \langle n|e^{iH_0t/\hbar}|\psi(t)\rangle = \langle n|\psi(t)\rangle_I$$
 (A.61)

where the subscript I indicates the interaction picture. The initial state $|\psi(t_0)\rangle_I = e^{iH_0t/\hbar} |m(t)\rangle = |m\rangle$. Inserting the states in Eq. (A.52), we find

$$\langle n|\psi(t)\rangle_{I} = \langle n|m\rangle + \frac{1}{i\hbar} \int_{t_{0}}^{t} \left\langle n|\hat{H}'_{I}(t')|m\rangle dt'$$

$$= \delta_{nm} + \frac{1}{i\hbar} \int_{t_{0}}^{t} e^{i(E_{n} - E_{m})t'/\hbar} \left\langle n|\hat{H}'(t')|m\rangle dt',$$
(A.62)

where we used the definition of an operator in the interaction picture in Eq. (A.44). Note that all expressions in the last line are given in the usual Schrödinger picture, which we worked with in the previous sections. The probability for a transition from the state $|m\rangle$ to the state $|n\rangle \neq |m\rangle$ is given by

$$P_{mn}(t) = \left| \frac{1}{i\hbar} \int_{t_0}^t dt' e^{i(E_n - E_m)t'/\hbar} \left\langle n|\hat{H}'(t')|m \right\rangle \right|^2 . \tag{A.63}$$

The first term in Eq. (A.62) corresponds to an unchanged quantum state $|m\rangle$, which has not been affected by any interaction. The second term describes one transition between two states induced by the Hamiltonian \hat{H}' :

- 1. We start with a quantum system in the eigenstate $|m\rangle$ of the Hamiltonian H_0 .
- 2. Then we evolve the quantum system in time from t_0 to t' using the Hamiltonian H_0 . Thus eigenstates $|m\rangle$ of H_0 do not change and only pick up a phase factor $\exp(iE_m(t'-t_0)/\hbar)$.
- 3. At time t', the Hamiltonian \hat{H}' affects the quantum system and leads to transitions between states, depending on the matrix elements $\langle n|\hat{H}'|m\rangle$.
- 4. After the interaction, the system is in a new state $|n\rangle$ and we evolve it with the Hamiltonian H_0 in time from t' to t and the quantum state picks up a phase factor $\exp(iE_n(t-t')/\hbar)$.
- 5. The transition probability is given by projecting this state at time t onto the eigenstates of H_0 . We explicitly include the phase factors from time evolution.

Higher order terms in Eq. (A.52) can be interpreted in the same way. The only difference is that there will be multiple transitions at different times t', t'', ..., and the quantum states between the transitions are evolved in time using the Hamiltonian H_0 leading to additional phase factors.

A.3 Green's function

Consider a differential equation of the form

$$L\psi(x) = f(x) \tag{A.64}$$

with a linear differential operator L = L(x). The Green's function G(x, y) of the differential operator is defined by

$$LG(x,y) = -\delta(x-y). \tag{A.65}$$

It can be used to obtained a general solution for the differential equation Eq. (A.64)

$$\psi(x) = -\int dy G(x, y) f(y) . \tag{A.66}$$

This is straightforward to see

$$L\psi(x) = L\left(-\int dy G(x,y)f(y)\right) = -\int dy LG(x,y)f(y) = \int dy \delta(x-y)f(y) = f(x). \quad (A.67)$$

A.4 Group theory

Symmetries are fundamental ingredients in describing physics. A symmetry transformation is a reversible operation which does not change the physical system. The set of symmetry transformations form a group.

Definition: A group G is a set of elements with an operation of multiplication that satisfies the following four properties:

- 1. Closure: $A, B \in G \Rightarrow AB \in G$
- 2. Associativity: $A, B, C \in G \Rightarrow (AB)C = A(BC)$
- 3. Identity: there is $E \in G$ such that AE = EA = A for all $A \in G$
- 4. Inverse: For all $A \in G$ there is $A^{-1}: AA^{-1} = E$

Examples include

- Trivial group: $\{E\}$
- Discrete Z_2 group $\{A, E\} \in Z_2$, $A = A^{-1}$ and thus $E = AA^{-1} = A^2$
- O(N) the orthogonal group: group of $n \times n$ orthogonal real matrices
- SO(N) the special orthogonal group: group of $n \times n$ orthogonal real matrices with unit determinant
- U(1) the unit complex numbers $\{e^{i\alpha}\}, \alpha \in \mathbb{R}$
- U(N) the unitary group: group of $n \times n$ complex unitary matrices
- SU(N) the special unitary group: group of $n \times n$ complex unitary matrices with unit determinant
- Lorentz group SO(3,1) with its spin group SL(2,C).

The first two examples are so-called discrete finite groups. The remaining examples are Lie groups, which are continuous groups. In fact all of them (apart from the Lorentz group) are compact. U(1), SU(N) and SO(N) are so-called simply Lie groups. The unitary group can be decomposed in terms of the special unitary group and the unit complex numbers: $U(N) \cong SU(N) \times U(1)$.

A.4.1 Lie groups

The connected component of Lie group which contains the identity can be described by the underlying Lie algebra. If A is an element in the Lie algebra, $\exp(\alpha A)$, $\alpha \in \mathbb{R}$ is a one-parameter family of group elements in the Lie group. The vector space of the Lie algebra can be described by the so-called "generators" which form a basis. Thus any element of the Lie algebra (and the connected component of the identity in the Lie group) can be described in terms of those generators. In physics we generally

use $\exp(i\alpha_i T^i)$ with real parameters α_i and hermitean matrices T^i . For example the generators of the spin group SU(2) are the Pauli matrices. For SU(3) they are the so-called Gell-Mann matrices. As SU(N) is a unitary group, the generators are hermitean matrices. In physics we typically normalize the generators as $\operatorname{tr}(T^a T^b) = \frac{1}{2} \delta^{ab}$.

A.4.2 Representations

Symmetries leave the system invariant, but transform states $|\psi\rangle \in \mathcal{H}$ in the Hilbert space. Representations are defined as mappings from the abstract group to linear transformations acting on a vector space which preserve the group structure. For example the group SU(2) can be represented by 2×2 special unitary matrices. In particular the generators are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{A.68}$$

We can however similarly construct a 3-dimensional representation by mapping the three generators of SU(2) to the matrices

$$J_{1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad J_{2} = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad J_{3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} . \tag{A.69}$$

A.4.3 Special relativitiy and the Lorentz group

The equivalence of inertial reference frames implies that space is isotropic and homogeneous and time is also homogeneous. It is not possible to distinguish inertial reference frames. In particular, light moves at the same speed in every reference frame F(F'): the distance travelled, $r^{(\prime)} = ct^{(\prime)}$. Hence $0 = -(ct)^2 + r^2 = -(ct')^2 + r'^2$ and more generally the interval s

$$s^{2} = -c^{2}t^{2} + x^{i}x^{i} = -c^{2}t'^{2} + x'^{i}x'^{i}$$
(A.70)

with $r^2 = x^i x^i = \sum_i (x^i)^2$ is the same in all inertial reference frames. Linear transformations which leave the interval s unchanged are known as Lorentz transformations.

We measure time in the same units as distance, i.e. c=1, and combine both of them in a 4-vector x^{μ} , $\mu=0,1,2,3$ with

$$x^0 = t$$
 and $(x^i) = \begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix}$ (A.71)

and thus the interval s is

$$s^2 = -x^0 x^0 + x^i x^i = \eta_{\mu\nu} x^{\mu} x^{\nu} \tag{A.72}$$

with the metric tensor

$$(\eta_{\mu\nu}) = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} . \tag{A.73}$$

From the condition that the interval s is invariant under Lorentz transformations $x'^{\mu} = \Lambda^{\mu}_{\nu} x^{\nu}$

$$\eta_{\mu\nu}x^{\prime\mu}x^{\prime\nu} = \eta_{\mu\nu}\Lambda^{\mu}_{\ \rho}\Lambda^{\nu}_{\ \sigma}x^{\rho}x^{\sigma} \equiv \eta_{\rho\sigma}x^{\rho}x^{\sigma} \tag{A.74}$$

it follows that Lorentz transformations satisfy

$$\eta_{\rho\sigma} = \eta_{\mu\nu} \Lambda^{\mu}_{\ \rho} \Lambda^{\nu}_{\ \sigma} \qquad \Leftrightarrow \eta = \Lambda^{T} \eta \Lambda \tag{A.75}$$

Taking the determinant we find that

$$\det \Lambda = \begin{cases} 1 & \text{proper Lorentz transformations} \\ -1 & \text{improper Lorentz transformations} \end{cases}$$
(A.76)

and the 00 component yields the condition $|\Lambda_0^0| \ge 1$. If $\Lambda_0^0 \ge 1 (\le -1)$ it is an orthochronous (non-orthochronous) Lorentz transformation. Thus the Lorentz group splits in 4 disconnected components

proper orthochronous
$$L_{+}^{\uparrow}$$
: det $\Lambda = 1, \Lambda_{0}^{0} \ge 1$ (A.77)

proper non-orthochronous
$$L_{+}^{\downarrow}$$
: det $\Lambda = 1, \Lambda_{0}^{0} \leq -1$ (A.78)

improper orthochronous
$$L_{-}^{\uparrow}$$
: det $\Lambda = -1, \Lambda_{0}^{0} \ge 1$ (A.79)

improper non-orthochronous
$$L_{-}^{\downarrow}$$
: det $\Lambda = -1, \Lambda_{0}^{0} \leq -1$ (A.80)

The set of events parameterized by x^{μ} coordinates together with the metric tensor $\eta_{\mu\nu}$ defines a space called the Minkowski space-time. Distances are invariant under Lorentz transformations

$$\Delta s^2 = \eta_{\mu\nu} (x^{\mu} - y^{\mu})(x^{\nu} - y^{\nu}) \qquad ds^2 = \eta_{\mu\nu} dx^{\mu} dx^{\nu}$$
 (A.81)

Indices are lowered and raised with $\eta_{\mu\nu}$ and $\eta^{\mu\nu}$ (the components of the inverse of the metric, η^{-1} . 4-vectors with an upper index x^{μ} are called contravariant vectors and with a lower index x_{μ} covariant (co-vary with the basis) vectors. Covariant vectors form the dual vector space to the contravariant vectors. A general mixed tensor transforms as

$$T_{\nu_1\nu_2...\nu_l}^{\prime\mu_1\mu_2...mu_k} = \Lambda_{\rho_1}^{\mu_1}\Lambda_{\rho_2}^{\mu_2}\dots\Lambda_{\rho_k}^{\mu_k}\Lambda_{\nu_1}^{\sigma_1}\Lambda_{\nu_2}^{\sigma_2}\dots\Lambda_{\nu_l}^{\sigma_l}T_{\sigma_1\sigma_2...\sigma_l}^{\rho_1\rho_2...\rho_k}.$$
(A.82)