Institut für Physik und Astronomie, Universität Potsdam
Wintersemester 2011/12

Quantenmechanik II
Grundbegriffe der Quantenfeldtheorie

Carsten Henkel

Baustelle 'Skriptum'

Diese Notizen sind in den Jahren 2006 und 2007 entstanden, in denen ich die Vorlesung Quanten II komplett gehalten habe. Hier gebe ich nur den dritten Teil zur Feldquantisierung wieder. Im WS 2011/12 bringe ich nicht alles in der Vorlesung. Nehmen Sie die Notizen als Anregung zum Nach- und Weiterlesen. Es gilt: kein Anspruch auf Vollständigkeit, und Fehler können überall auftreten.

- Einführung in die Quantenfeldtheorie
  → Kapitel 3: Phononen auf diskretem Gitter, kanonische Quantisierung, skalares, relativistisches Feld (Klein-Gordon-Feld), Zerfall von Teilchen, Quantisierung von Fermionen, Pauli-Prinzip und Vielteilchen-Theorie, Konzepte der Supraleitung

- zeitabhängige Störungstheorie
  → Anhang A: Zeitentwicklungsoperator, Fermis Goldene Regel

Chapter 3

Field Quantization

The general idea of field quantization is: we promote field amplitudes to operators acting on a suitable Hilbert space. In the context of quantum mechanics (more precisely: wave mechanics), Schrödinger's wave function plays the role of the field. Promoting it to an operator is called 'second quantization' for historical reasons. In the case of electrodynamics which is already a field theory, the same procedure could be called 'first quantization'.

Classical mechanics	Wave mechanics	Quantum field theory QFT
point particles	wave packet	elementary excitations
coordinates q, p	operators $\hat{q}$, $\hat{p}$	
	or q, $-\mathrm{i}\hbar\frac{\partial}{\partial q}$	
	wave function ψ	field operator $\hat{\psi}$
classical path	wave packet	particle creation/annihilation
Geometrical optics	Electrodynamics	Quantum Electrodynamics
light rays	classical fields E, B	field operators $\hat{E}$, $\hat{B}$
		photons

Table 3.1: Hierarchy of theories in physics

3.1 Why QFT?

- observation: creation and decay of particles (in pairs, into other particles)

- theoretical reason: "second quantization" of quantum mechanics as a field theory and of electrodynamics (Dirac 1927[1])
- efficient representation of quantum many-body systems ("quasi-particles")

What QFT is good for

Elementary particles

- the Standard Model is a QFT
- particle = "elementary excitation of a field mode" (W. Lamb)
  field mode = global oscillation pattern with frequency ω_k, spatial distribution (plane wave, standing wave etc.), polarization, charge ...
  excitation energy: quantized in "packets" $\hbar\omega_k$ (Einstein, de Broglie)
- these particles/fields live in "vacuum" (no ether, no other material background)

Many-body physics

- semi-conductor, metal, quantum liquids, elastic crystal
- quasi-particle = elementary excitation of normal mode of an extended (coupled) system
  example: phonons (quantized version of elastic waves)
- these quasi-particles live on a matter background

Particles are surrounded by "clouds" of other particles

- *example*: electron in a metal is "screened" by positive charge from depletion (Coulomb repulsion). Net charge from "far away" is reduced
- *example*: relativistic electron is surrounded by "virtual photons". This changes its mass and increases its charge. At the energy scale $90\,\mathrm{GeV}$ of the electroweak interactions, the fine structure constant has increased to $\approx 1/127$
- this leads to effective interactions via the exchange ("overlap") of the clouds around two particles. *Example*: van der Waals interaction between two atoms (neutral, no average dipole moment), between colloid particles, nano-dust ... Fritz London 1930[2]: explains this from

[1] "The Quantum Theory of the Emission and Absorption of Radiation", P. A. M. Dirac, *Proc. Roy. Soc.* (*London*) *A* **114** (1927) 243

[2] "Zur Theorie und Systematik der Molekularkräfte", F. London, *Z. Phys.* **63** (1930) 245

quantum fluctuating dipole moments that are correlated by electrostatic fields.

→ the "renormalization program" of QFT: to extract finite and measurable quantities from infinite integrals (self-energy, mass shift ...)

3.2 QFT at work

Electron and positrons: Dirac field operator

Operator for electrons and positrons (field operator of the "Dirac theory" = relativistic quantum mechanics of electron)

$$\hat{\Psi}(x) = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \sum_\sigma \left(u_{\mathbf{k}\sigma}\, \mathrm{e}^{-\mathrm{i}k\cdot x} \hat{a}_{\mathbf{k}\sigma} + v_{\mathbf{k}\sigma}\, \mathrm{e}^{\mathrm{i}k\cdot x} \hat{b}^\dagger_{\mathbf{k}\sigma} \right) \tag{3.1}$$

This is a spinor operator with four components. The spinor solution $u_{\mathbf{k}\sigma}$ is the one discussed in relativistic quantum mechanics, it corresponds to a positive frequency solution because $k \cdot x = \omega_k t - \mathbf{k}\cdot\mathbf{x}$ with $\omega_k = +E(k)/\hbar$. The negative energy solution ("positron") $v_{\mathbf{k}\sigma}$ appears as well.

- the amplitudes of the plane wave modes become operators:

The operator $a_{\mathbf{k}\sigma}$ *annihilates* an electron in the mode $u_{\mathbf{k}\sigma}$: energy $E(k)$, momentum $\hbar\mathbf{k}$, spin σ. The operator $b^\dagger_{\mathbf{k}\sigma}$ *creates* a positron in the mode $v_{\mathbf{k}\sigma}$: energy $E(k)$, momentum $\hbar\mathbf{k}$, spin σ .... The positron created by $b^\dagger_{\mathbf{k}\sigma}$ can also be understood as a "missing electron" in the Fermi sea of occupied states with negative energy.

What is this field operator good for? To represent the interactions between particles as an operator that creates/annihilates/converts particles. In many-body applications, it serves to construct the particle density, the current density etc.

The Hilbert space of QFT: Fock space

Pick one mode $\mathbf{k}\sigma$ and consider $a = a_{\mathbf{k}\sigma}$ and $a^\dagger = a^\dagger_{\mathbf{k}\sigma}$. (*Note*: electrons and positrons correspond to different modes.) These are *ladder operators*, as illustrated in Fig.3.1.

The starting point to construct the Fock-Hilbert space is the *vacuum state* $|0\rangle = |\mathrm{vac}\rangle$ where no particles are present, i.e. all field modes are in their lowest excitation state. The vacuum state has the property

$$a|\mathrm{vac}\rangle = 0 \tag{3.2}$$

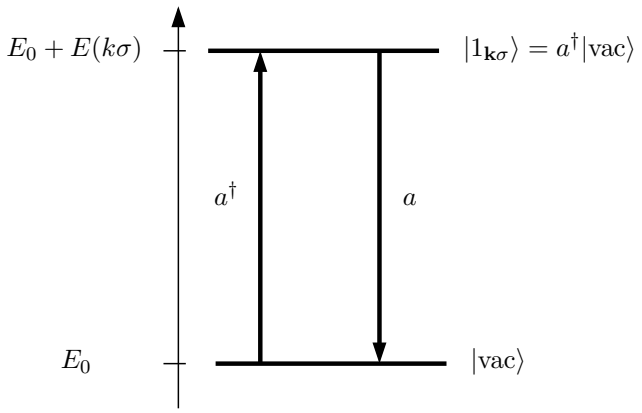

Figure 3.1: Creation and annihilation operators ($a^\dagger$ and a) as ladder operators.

copied from the ground state of a harmonic oscillator in quantum mechanics. Do not mix up the zero vector 0 (it has norm zero, as it must in a vector space) with the vacuum state vector $|0\rangle$. We use the notation $|\mathrm{vac}\rangle$ to avoid the confusion.

If the creation operator is applied on the vacuum, we get another state

$$a^\dagger|\mathrm{vac}\rangle = |1_{\mathbf{k}\sigma}\rangle \tag{3.3}$$

where the notation means: "One quantum of excitation in the mode characterized by the quantum numbers $\mathbf{k}\sigma$." The energy of this state is $E(k)$ above the energy of the vacuum state (denoted E_0 in Fig.3.1). The change in energy can also be expressed as the "ladder identity" (copied from QM I):

$$\left[\hat{H}, \hat{a}\right] = -E(k)\hat{a} \tag{3.4}$$

where the operator H gives the energies of the quantum states.

For the electron (and positron), this procedure does not continue because of the Pauli principle: no two electrons can occupy the same quantum state. Or in our field mode language: "A field mode of the electronc field is either carrying zero excitation or one."

Mathematically, this is implemented by postulating the operators a and $a^\dagger$ anti-commute:

$$\{a, a^\dagger\} = 1 \quad \text{with} \quad \{A, B\} = AB + BA \tag{3.5}$$

$$\{a^\dagger, a^\dagger\} = 0, \qquad \{a, a\} = 0 \tag{3.6}$$

The first commutator is formally similar to the one you know from the harmonic oscillator, apart from the fact that it is an anticommutator. The

other two expressions give non-trivial information for the electron operators. They imply that a is "nilpotent" or $a^\dagger a^\dagger = 0$. This corresponds to the Pauli principle.

The quantized Dirac field is also made from anti-commuting operators. This implies that many-electron wave functions (to be defined in Sec.3.7.1 below) is anti-symmetric under an exchange of electron coordinates. This is called "Fermi-Dirac statistics" – and the fundamental reason for this comes from QFT and the fact that the electron has a spin $1/2$. This is one aspect of the

> *Spin Statistics Theorem*. Particles with half-integer spin (electrons, quark ...) satisfy Fermi-Dirac statistics and are represented by creation and annihilation operators that anti-commute.
> Particles with integer spin (Higgs boson, photon, gluons, mesons ...) satisfy Bose-Einstein statistics and their mode operators obey commutation relations.

One-particle sector. Now go back and take into account all modes. The so-called "one-particle sector" $\mathcal{H}_1$ of the Fock-Hilbert space is spanned by all one-particle states:

$$\mathcal{H}_1 = \mathrm{span}\{|1_{\mathbf{k}\sigma}\rangle, \mathbf{k}\sigma = \ldots\} \tag{3.7}$$

where all complex linear combinations appear. This is, obviously, a quite large Hilbert space. It is in fact isomorphic to the space of the classical field theory: any linear combination of modes can be mapped to a linear combination of basis states. In this way, one can also make states that are correctly normalized. We have actually cheated in Eq.(3.5) because the number 1 actually corresponds to the L^2-norm of the classical mode function – which is infinite for a plane wave.

Take an L^2-integrable solution of the classical field theory and from its Fourier coefficients $\tilde{\phi}_\sigma(\mathbf{k})$ construct the operator

$$a_\phi = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \sum_\sigma \tilde{\phi}_\sigma(\mathbf{k}) a_{\mathbf{k}\sigma} \tag{3.8}$$

and its adjoint $a_\phi^\dagger$. Then the (anti)commutation relations give (exercise)

$$\{a_\phi, a_\phi^\dagger\} = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \sum_\sigma |\tilde{\phi}_\sigma(\mathbf{k})|^2 \tag{3.9}$$

provided the relation (3.5) is generalized to

$$\{a_{\mathbf{k}\sigma}, a^\dagger_{\mathbf{k}'\sigma'}\} = (2\pi)^3\delta(\mathbf{k}-\mathbf{k}')\delta_{\sigma\sigma'} \tag{3.10}$$

The integral in Eq.(3.9) is now simply the L^2-norm of the classical solution which can be set equal to one. The previous relations are thus valid for creation and annihilation operators that are defined with respect to suitable "wavepackets".

N-particle sector. The preceding construction continues by applying products of mode operators $a^\dagger_{\mathbf{k}\sigma}\dots a^\dagger_{\mathbf{k}'\sigma'}$ to the vacuum state. This gives states with higher and higher particle number.

Reminder: harmonic oscillator, two degrees of freedom

$$H = \frac{p_a^2}{2m} + \frac{K}{2}q_a^2 + \frac{p_b^2}{2m} + \frac{K}{2}q_b^2 \tag{3.11}$$

eigenfrequencies $\omega_a = \omega_b = \sqrt{K/m}$. Quantization in terms of creation and annihilation operators:

$$q_a = \sqrt{\frac{\hbar}{2m\omega_a}}\left(a + a^\dagger\right), \qquad p_a = -\mathrm{i}\sqrt{\frac{\hbar m\omega_a}{2}}\left(a - a^\dagger\right) \tag{3.12}$$

$$a = \sqrt{\frac{m\omega_a}{2\hbar}}\left(q_a + \frac{\mathrm{i}}{m\omega_a}p_a\right), \qquad a = \sqrt{\frac{m\omega_a}{2\hbar}}\left(q_a - \frac{\mathrm{i}}{m\omega_a}p_a\right) \tag{3.13}$$

and b, $b^\dagger$ for q_b, p_b. Commutation relations

$$\left[a,\, a^\dagger\right] = 1, \qquad \left[b,\, b^\dagger\right] = 1 \tag{3.14}$$

all others are zero.

'Number operator' $a^\dagger a$ counts excitations. In quantum field theory, an excitation is interpreted as a particle, and $a^\dagger a$ counts particles with quantum numbers (mode function, spin etc.) specific to the oscillator of type 'a'. In other words: a 'particle' is an excitation of a 'normal mode' of a field that behaves like a harmonic oscillator. The operators $a^\dagger$ and a implement the creation/annihilation of this particle.

3.3 Basics: phonons

This is a simple model from classical mechanics to start with. We avoid technical complications and work with a system made up of discrete oscillators and of finite size. The basic observation that we are going to make:

the 'small amplitude vibrations' of classical mechanics become the 'modes' of a 'field' whose dispersion relation is similar to that of a relativistic particle.

3.3.1 Hamiltonian

Hamiltonian:

$$H = \sum_n \frac{p(x_n)^2}{2m} + \sum_n \frac{K}{2}\left[q(x_n + a) - q(x_n)\right]^2 + \sum_n \frac{m\Omega^2}{2} q(x_n)^2 \qquad (3.15)$$

Here, the oscillator displacement is $q(x_n)$, its equilibrium position is x_n. The conjugate momentum is $p(x_n)$. The first term in (3.15) is the kinetic energy, the second the potential energy from the restoring force to equilibrium (spring constant $m\Omega^2$), and the third the potential energy from linear coupling to the neighboring oscillator, with spring constant K. The oscillators are separated by the discrete lattice vector a – this is a one-dimensional chain. The sum runs over N oscillators in total. We take periodic boundary conditions: $q(x_{n+N}) = q(x_n + Na) = q(x_n)$.

In classical mechanics, $q_n \equiv q(x_n)$ and $p_{n'}$ are canonically conjugate. This means that the Poisson brackets are $\{q_n,\, p_{n'}\} = \delta_{nn'}$.

We promote this to a quantized theory by a recipe called 'canonical quantization': replace Poisson brackets by commutators. In other words: we promote coordinates and conjugate momenta to operators that do not commute:

$$[q_n,\, p_{n'}] = \mathrm{i}\hbar\delta_{nn'}, \qquad [q_n,\, q_{n'}] = 0, \qquad (3.16)$$

of course, the momenta commute also with themselves.

The time evolution of observables follows in the quantized theory from the Heisenberg equations, for example:

$$\frac{\mathrm{d}q_n}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}\left[H,\, q_n\right] \qquad (3.17)$$

with Hamilton operator H obtained from (3.15) written with operators. In classical mechanics, we have the same equation written in terms of Poisson brackets.

3.3.2 Mode expansion

The system is periodic, therefore it is useful to make a Fourier expansion:

$$q(x) = \sum_{k\in \mathrm{BZ}} \tilde{q}(k)\mathrm{e}^{\mathrm{i}kx}, \qquad \tilde{q}(k) = \frac{1}{N}\sum_n q(x_n)\mathrm{e}^{-\mathrm{i}kx_n} \qquad (3.18)$$

and similarly for $p(x_n)$. The discrete wave vectors k run from $-\pi/a$ to π/a in steps of $2\pi/L$ where $L = Na$ is the length of the chain. These points make up the 'Brillouin zone' BZ. Since the operator q is hermitean, one must have $\tilde{q}(-k) = \tilde{q}^\dagger(k)$. The commutation relations become

$$\left[\tilde{q}(k),\, \tilde{p}^\dagger(k')\right] = \frac{\mathrm{i}\hbar}{N^2} \sum_n \mathrm{e}^{\mathrm{i}(k-k')x_n} \tag{3.19}$$

Now for discretized wave vectors in the first Brillouin zone, $-\pi/a < k \leq \pi/a$, this sum of exponentials is nonzero only if $k - k' = 0 \mod 2\pi/a$. In addition, the difference of k-vectors is limited to $|k - k'| \leq 2\pi(N-1)/N$. Hence only for $k = k'$, the sum gives a nonzero result (which is trivially equal to N). So we have

$$\left[\tilde{q}(k),\, \tilde{p}^\dagger(k')\right] = \frac{\mathrm{i}\hbar}{N} \delta_{kk'} \tag{3.20}$$

with a Kronecker for the discrete wavenumbers.

A similar calculation gives for the Hamiltonian (see Exercise)

$$H = N \sum_{k\in \mathrm{BZ}} \frac{1}{2m} \tilde{p}^\dagger(k)\tilde{p}(k) + N \sum_k \left(\frac{m\Omega^2}{2} + K(1-\cos ka) \right) \tilde{q}^\dagger(k)\tilde{q}(k) \tag{3.21}$$

The key observation is that this is a sum of independent oscillators: one for each value of k. In classical terms: we have found the 'normal modes' of the system. But these modes provide also one basic recipe for field quantization: find the 'modes' that bring the Hamiltonian into a diagonal form[3] and promote the amplitudes of these modes to operators.

We note that the frequency for a mode with wavenumber k is given by

$$\omega_k^2 = \Omega^2 + \frac{2K}{m}(1-\cos ka) \approx \Omega^2 + c^2k^2 \tag{3.22}$$

In the last line, we have introduced the large-wavelength limit $ka \ll 1$ and expanded the cosine. This looks like the dispersion relation for a particle with rest mass Ω, with the speed of light being replaced by the 'speed of sound' $c^2 = Ka^2/m$. This is indeed the speed of long-wavelength oscillations that propagate on the chain. In the limit $\Omega \to 0$, one gets the linear dispersion $\omega_k = c|k|$ similar to light waves or sound waves.

[3] This could have been done at the classical level, of course.

3.3.3 Quantization

For each k, we have a harmonic oscillator and quantize in terms of the creation and annihilation operators

$$a_k = \sqrt{\frac{Nm\omega_k}{2\hbar}}\left[\tilde{q}(k) + \frac{\mathrm{i}}{m\omega_k}\tilde{p}(k)\right], \qquad a_k^\dagger = \sqrt{\frac{Nm\omega_k}{2\hbar}}\left[\tilde{q}^\dagger(k) - \frac{\mathrm{i}}{m\omega_k}\tilde{p}^\dagger(k)\right]. \tag{3.23}$$

One can check that the commutation relations are indeed those for independent oscillators

$$\left[a_k,\, a_{k'}^\dagger\right] = \delta_{kk'} \tag{3.24}$$

Hamiltonian (3.21) becomes

$$H = \sum_{k\in\mathrm{BZ}} \frac{\hbar\omega_k}{2}\left(a_k^\dagger a_k + a_k a_k^\dagger\right) = \sum_k \hbar\omega_k\left(a_k^\dagger a_k + \tfrac{1}{2}\right) \tag{3.25}$$

which is the usual form for the energy of a collection of independent oscillators. This kind of result one always gets when a field is quantized. The real benefit of the quantization procedure is the following 'mode expansion' of the particle displacement that is now operator-valued:

$$q(x,t) = \sum_{k\in\mathrm{BZ}} \sqrt{\frac{\hbar}{2m\omega_k N}}\left(a_k(t)\mathrm{e}^{\mathrm{i}kx} + a_k^\dagger(t)\mathrm{e}^{-\mathrm{i}kx_n}\right) \tag{3.26}$$

The t-dependence of the annihilation and creation operators is simple: multiply with $\mathrm{e}^{\pm\mathrm{i}\omega_k t}$.

We now discuss some applications. The physics behind this result is related to 'phonons'. These quasiparticles correspond to the excitations of the normal modes we just found. A typical stationary state of the system is specified by a set of occupation numbers $\{n_k\}$, one for each plane-wave mode $k \in \mathrm{BZ}$. In this state, one says that a number n_k of phonons make up the excitation of the mode k. There is no contradiction in having many phonons exciting a given mode: phonons are 'bosons' that are not subject to Pauli's exclusion principle.

3.3.4 Applications

Zero-point oscillations

The ground state of the quantized oscillator chain is characterized by the equations $a_k|\mathrm{vac}\rangle = 0$. Equivalently, $n_k = 0$ for all normal modes k. The mean value of the displacement in the ground state is zero:

$$\langle q(x)\rangle_{\mathrm{vac}} = \sum_{k\in\mathrm{BZ}} (\cdots)\langle a_k\rangle_{\mathrm{vac}} \tag{3.27}$$

because $\langle a_k \rangle_{\rm vac} = 0$ in the ground state (in any stationary state, in fact).

But the variance of $q(x)$ is not zero: this is related to the zero-point fluctuations of each phonon mode being a quantized harmonic oscillator. These zero-point oscillations can be detected with scattering experiments. We single out artificially one oscillator from the chain and compute the amplitude for a scattered wave with a wave vector transfer p:

$$\langle \mathrm{e}^{\mathrm{i}pq_n} \rangle = \mathrm{e}^{-\frac{1}{2}p^2 \langle q_n^2 \rangle}$$

This result is correct for a gaussian statistics[4] of the variable q_n. This average amplitude can be measured by letting the scattered wave interfere with a reference wave. The diffraction of X-rays by a crystal also leads to a similar behaviour of the intensities diffracted into a given order. In that case, p is the wave vector transfer of the diffraction peak.

The computation of the variance gives

$$\begin{aligned} \langle q_n^2 \rangle_{\rm vac} &= \sum_k \frac{\hbar}{2m\omega_k N} \langle a_k \mathrm{e}^{\mathrm{i}kx_n} a_k^\dagger \mathrm{e}^{-\mathrm{i}kx_n} \rangle_{\rm vac} \\ &= a \int_{\rm BZ} \frac{\mathrm{d}k}{2\pi} \frac{\hbar}{2m\omega_k}, \end{aligned} \tag{3.28}$$

where we used the standard rule of replacing a sum over k into an integral for a system with large length $L = Na$. This integral has some value that depends on $\Omega a/c$:

$$\langle q_n^2 \rangle_{\rm vac} = \frac{\hbar a}{2mc} \int_{-\pi}^{\pi} \frac{\mathrm{d}x}{2\pi} \left[(\Omega a/c)^2 + 2(1 - \cos x) \right]^{-1/2} \tag{3.29}$$

The integral is plotted in Figure 3.2. The long-wavelength approximation, $\omega_k^2 = \Omega^2 + c^2 k^2$ gives the dashed line which is in good overall agreement. We shall use this approximation in the following because it simplifies the calculations.

Three-dimensional case

We generalize to three dimensions: now, the number N of oscillators scales with volume L^3 of the system. The sum over $\mathbf{k}$ runs over a 3D Brillouin zone. The phonon dispersion relation for a simple cubic lattice is given by

$$\omega_{\mathbf{k}}^2 = \Omega^2 + \frac{2K}{m} \left(3 - \cos k_x a - \cos k_y a - \cos k_z a \right) \approx \Omega^2 + c^2 \mathbf{k}^2 \tag{3.30}$$

[4] We are a cheating a little bit, since q_n is in fact an operator, but one can introduce a 'quasi-distribution' that is indeed gaussian in the ground state (and at finite temperature as well).

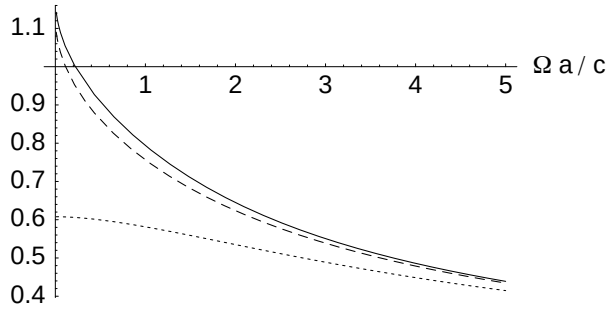

Figure 3.2: Two upper curves: integral in Eq.(3.29) as a function of $\Omega a/c$. The limiting value for $\Omega \to 0$ is ≈ 1.18. The dashed line corresponds to the approximation $1 - \cos x \approx x^2/2$ under the integral. Dotted line: 3D equivalent.

with the sound velocity $c^2 = Ka^2/m$ as before. In the long-wavelength limit, the dispersion relation is isotropic.

A similar calculation leads to the zero-point fluctuations

$$\langle q_n^2 \rangle_{\rm vac} = a^3 \int\limits_{\rm BZ} \frac{{\rm d}^3 k}{(2\pi)^3} \frac{\hbar}{2m\omega_k} \tag{3.31}$$

Let us make an approximation that is often used, and consider a spherical Brillouin zone with the same number of points/the same volume. Its radius $k_{\rm max}$ is fixed by

$$\frac{4\pi}{3} k_{\rm max}^3 = \left(\frac{2\pi}{a} \right)^3 \tag{3.32}$$

where the right hand side is the number of points in the 'Brillouin cube' of the 3D cubic lattice. We write $k_{\rm max} = \omega_{\rm D}/c$ in terms of the so-called Debye frequency $\omega_{\rm D}$. This quantity is often used as an high-frequency cutoff for the phonon spectrum. Typical values of the Debye frequency are of order $10^{12}\,{\rm s}^{-1}$, depending on the crystal lattice constant and stiffness.

Hence, with this approximation:

$$\langle q_n^2 \rangle_{\rm vac} = \frac{\hbar a^3}{2m} 4\pi \int\limits_0^{k_{\rm max}} \frac{k^2 {\rm d}k}{(2\pi)^3} \omega_k^{-1} \tag{3.33}$$

which gives another integral that depends on $\Omega a/c$ (left as an exercise). Making the long-wavelength approximation and taking a spherical Brillouin zone, the resulting zero-point fluctuation is plotted as a dotted line in Figure 3.2. The fluctuation is normalized to $\hbar a/(2mc)$, as in Eq.(3.29).

Specific heat

We are now going to make some thermodynamics. Recall the quantum thermodynamics for a single oscillator: the free energy is given by

$$\mathcal{F} = (1/\beta)\log[2\sinh(\beta\hbar\omega/2)] \tag{3.34}$$

with $1/\beta = k_B T$ and the specific heat (per degree of freedom) is found from

$$C = \frac{\partial}{\partial T}\frac{\partial}{\partial \beta}(\beta\mathcal{F}) \tag{3.35}$$

(One differentiates the mean energy with respect to temperature.)

Now, the harmonic chain is a collection of oscillators with frequencies ω_k. In thermodynamic equilibrium, we assume that each normal mode is specified by a thermal distribution. All normal modes are independent, hence the total free energy is the sum of free energies:

$$\mathcal{F} = \sum_k (1/\beta)\log 2\sinh(\beta\hbar\omega_k/2) = \frac{a^3 N}{\beta}\int\limits_{BZ}\frac{\mathrm{d}^3 k}{(2\pi)^3}\log 2\sinh(\beta\hbar\omega_k/2) \tag{3.36}$$

This is proportional to the volume $a^3 N$ of the system, as it should be for the extensive quantity 'free energy'. We thus define a density of free energy $f = \mathcal{F}/a^3 N$.

This free energy density contains a zero-point contribution plus a thermal one. We compute first the zero-point contribution for a linear dispersion $\omega_k = c|\mathbf{k}|$:

$$\begin{aligned} f(T\to 0) &= \frac{4\pi}{\beta}\int\limits_0^{k_{\max}}\frac{k^2\mathrm{d}k}{(2\pi)^3}\frac{\beta\hbar\omega_k}{2} \\ &\approx 2\pi\hbar c\int\limits_0^{k_{\max}}\frac{k^3\mathrm{d}k}{(2\pi)^3} = \frac{\hbar c k_{\max}^4}{(4\pi)^2} \sim \frac{\hbar c}{a^4} \end{aligned} \tag{3.37}$$

This is temperature-independent (by construction), hence it does not contribute to the specific heat. The result (3.37) corresponds to the energy of one phonon at the edge of the Brillouin zone, $\hbar c/a \sim \hbar\omega_D$, per unit cell of the crystal. Of course, this zero-point energy is not directly observable, one would have to destroy the crystal to see it. But sometimes corrections due to finite surface size, thickness and so on appear that can be measured as "Casimir forces". However, the main field that contributes in that context

is the electromagnetic one, not the phonon field.[5]

Finally, the temperature-dependent part of the free energy is the one that is relevant for the specific heat (3.35) as well. This was pointed out and calculated by Einstein and Debye, using different models for the distribution of phonon frequencies. With our simple model $\omega_k = c|\mathbf{k}|$, we get

$$\begin{aligned} f(T) - f(0) &\approx \frac{4\pi}{\beta} \int_0^{k_{\max}} \frac{k^2 \mathrm{d}k}{(2\pi)^3} \log(1 - \mathrm{e}^{-\beta\hbar c k}) \\ &\approx \frac{1}{\beta^4 \hbar^3 c^3} \frac{4\pi}{(2\pi)^3} \int_0^{\beta\hbar\omega_D} x^2 \mathrm{d}x \log(1 - \mathrm{e}^{-x}) \end{aligned} \tag{3.38}$$

This result is plotted in Figure 3.3 in units of $(\beta^4\hbar^3c^3)^{-1}$ as a function of

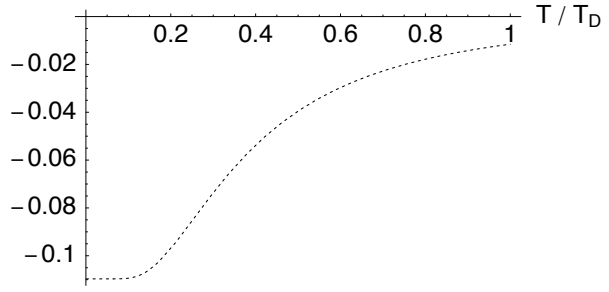

Figure 3.3: Free energy per unit volume of a harmonic lattice in 3D, Eq.(3.38), in units of $(\beta^4\hbar^3c^3)^{-1}$ and as a function of $T/T_D = (\beta\hbar\omega_D)^{-1}$. The phonon dispersion relation is approximated as $\omega_k = c|\mathbf{k}|$. The value for $T \to 0$ is $-\pi^2/90 \approx -0.11$.

the scaled temperature $(\beta\hbar\omega_D)^{-1} = k_BT/\hbar\omega_D$ (Debye temperature typically $\hbar\omega_D/k_B \sim 300\,\mathrm{K}$). At low temperatures, $k_BT \ll \hbar\omega_D$, the integral is constant. In this regime, the free energy (3.38) scales like $1/\beta^4 = T^4$. It follows, that the specific heat (3.35) per volume is proportional to T^3 in this regime. This is an important result that can be directly compared to experiments. As the temperature increases, the dependence is getting more complicated. In this 'classical regime', our linear chain is in fact no longer a realistic model because nonlinear contributions to the oscillations of the crystal play a role.

[5] More precisely, the change in electromagnetic zero-point energy per unit area for a pair of perfectly reflecting plates with distance a scales like Eq.(3.37), with c being the speed of light.

3.4 Relativistic bosons

Klein-Gordon field

We now summarize a few important properties of the quantization of the Klein-Gordon field. With respect to the phonons, we are going to consider a continuous, position-dependent quantum operator $q(x)$ or $\Phi(x)$. In addition, we have to ensure that the quantization is compatible with special relativity.

3.4.1 Continuum limit

Let us first comment on the limit that the chain of oscillators merges into a continuous field (an 'elastic string'). We shall base the discussion on the Lagrangian formulation, and our goal will be a prescription to get the following Lagrangian for the Klein-Gordon field (see lectures on relativistic quantum mechanics)

$$L = \int \mathrm{d}^3x \left[\frac{1}{2}(\partial_t \Phi)^2 - \frac{c^2}{2}(\nabla\Phi)^2 - \frac{1}{2}(mc^2/\hbar)^2\Phi^2 \right] \tag{3.39}$$

Compared to the previous formulation, this is only valid for a real-valued field $\Phi(\mathbf{x}, t)$.

The Lagrangian for the linear chain whose Hamiltonian is (3.15) reads, generalizing to three dimensions:

$$L = \sum_{\mathbf{x}} \left[\frac{M}{2}\dot{q}(\mathbf{x})^2 - \frac{M\Omega^2}{2}q(\mathbf{x})^2 - \frac{K}{2}\sum_i \left(q(\mathbf{x}+\mathbf{a}_i) - q(\mathbf{x})\right)^2 \right] \tag{3.40}$$

Here, we have written M for the oscillator mass to avoid confusion with the mass m in the Klein-Gordon field. The vectors $\mathbf{a}_i$ correspond to the directions and distances for the coupling between neighboring oscillators. The natural replacement rule to go from the summation over $\mathbf{x}$ to an integral is, of course:

$$\sum_{\mathbf{x}} \mapsto \int \frac{\mathrm{d}^3x}{a_x a_y a_z} \tag{3.41}$$

We see that the mass density $\rho \equiv M/(a_x a_y a_z)$ can be factored from the Lagrangian. Note that this common factor does not change the Euler-Lagrange equations (principle of least action). We extend $q(\mathbf{x}, t)$ to a continuous function and get

$$L \mapsto \rho \int \mathrm{d}^3x \left[\frac{1}{2}(\partial_t q)^2 - \frac{\Omega^2}{2}q^2 - \frac{K}{2M}\sum_i \left(q(\mathbf{x}+\mathbf{a}_i) - q(\mathbf{x})\right)^2 \right] \tag{3.42}$$

Finally, in the limit $a \to 0$ (at fixed ρ), we expand $q(\mathbf{x} + \mathbf{a}_i)$ in the coupling between neighbors and get

$$[q(\mathbf{x} + \mathbf{a}_i) - q(\mathbf{x})]^2 = \mathbf{a}_i^2 \left(\frac{\partial q}{\partial x_i} \right)^2 \tag{3.43}$$

where the coordinate x_i is chosen along the direction of $\mathbf{a}_i$. We shall take the simplest case that $|\mathbf{a}_i| = a$ in three orthogonal directions (cubic lattice) so that

$$\sum_i \mathbf{a}_i^2 \left(\frac{\partial q}{\partial x_i} \right)^2 = a^2 (\nabla q)^2 \tag{3.44}$$

With the definition for the speed of light/sound, $c^2 = Ka^2/M$, and the replacement $\Omega \mapsto mc^2/\hbar$, we thus get the Klein-Gordon Lagrangian (3.39) if we identify the Klein-Gordon field $\Phi(\mathbf{x}, t) = \sqrt{\rho} q(\mathbf{x}, t)$.

In the continuum limit $a \to 0$, the dispersion relation (3.22) also becomes identical to the relativistic one:

$$\omega_k^2 = \Omega^2 + \frac{c^2}{2a^2} \left(3 - \sum_i \cos k_i a \right) \to (mc^2/\hbar)^2 + c^2 \mathbf{k}^2. \tag{3.45}$$

We thus have formulated a 'mechanical model' for the propagation of a relativistic field. Of course, the modern interpretation of the field dynamics does no longer mention the underlying oscillators, be they discrete or continuous. The Klein-Gordon field 'lives' in empty space. This empty space behaves like a rigid medium in the sense that the field amplitude at every space point corresponds to a harmonic oscillator with frequency $\Omega = mc^2/\hbar$. This is a very large frequency already for the electron mass.

3.4.2 Quantization

We now apply the rules for the continuum limit to translate the quantized phonon field to the relativistic case. From hereon, we put $\hbar = c = 1$.

Field operator

In the discrete summations over the Brillouin zone, the spacing of the k-vectors can be first kept the same ($2\pi/L$), if we continue to work with a finite 'quantization volume' and periodic boundary conditions.[6] The upper limit of the Brillouin zone, π/a, is going to infinity in the continuum limit.

[6] This can be relaxed and the theory formulated in an infinite volume. The price to pay is that the a_k become operator-valued distributions that make sense only when smeared out with L^2-integrable functions.

Hence we now have a countable, but infinite set of plane-wave modes in the expansion of the phonon displacement operator:

$$q(\mathbf{x},t) = \sum_{\mathbf{k}\in \mathrm{BZ}} \frac{1}{\sqrt{2M\omega_k N}} \left(a_k(t) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} + a_k^\dagger(t) \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \right) \tag{3.46}$$

We write $MN = (M/a^3)Na^3 = \rho V$ and see that q involves the scale factor $1/\sqrt{\rho}$. For the time-dependent Klein-Gordon operator, $\Phi(x) = \sqrt{\rho} q(x)$, we thus have

$$\Phi(x) = \sum_{\mathbf{k}\in \mathrm{BZ}} \frac{1}{\sqrt{2\omega_k V}} \left(a_k \mathrm{e}^{-\mathrm{i}k_\mu x^\mu} + a_k^\dagger \mathrm{e}^{\mathrm{i}k_\mu x^\mu} \right) \tag{3.47}$$

using the obvious 4-momentum $k_\mu = (\omega_k, -\mathbf{k})$ and the time evolution of the Heisenberg operators $a_k(t)$.

Energy and momentum operators

The quantized Hamiltonian still has the same form

$$H = \sum_{\mathbf{k}\in \mathrm{BZ}} \omega_k \left(a_\mathbf{k}^\dagger a_\mathbf{k} + \frac{1}{2} \right) \tag{3.48}$$

For each excitation in mode $\mathbf{k}$, the energy increases by an amount ω_k. This corresponds to the idea that particles in quantum field theory are viewed as excitations of (continuous) fields. More formally, we have the relation

$$\left[H, a_\mathbf{k}^\dagger \right] = \omega_k a_\mathbf{k}^\dagger \tag{3.49}$$

From this, we can derive that by acting with a creation operator on the vacuum state, $a_\mathbf{k}^\dagger|\mathrm{vac}\rangle$, one gets a state with an energy ω_k above the vacuum state. This is compatible with the interpretation: '$a_\mathbf{k}^\dagger$ creates a particle with momentum $\mathbf{k}$'.

The vacuum is defined by the absence of any particle, $a_\mathbf{k}|\mathrm{vac}\rangle = 0$. This suggests to subtract the zero-point energy in the Hamiltonian (3.48): one thus works with $H \mapsto H - \langle \mathrm{vac}|H|\mathrm{vac}\rangle$ or so-called 'normally ordered' operators (this operator ordering is expressed by the notation $: \ldots :$)

$$H \mapsto \sum_{\mathbf{k}\in \mathrm{BZ}} \frac{\omega_k}{2} :\!\left(a_\mathbf{k}^\dagger a_\mathbf{k} + a_\mathbf{k} a_\mathbf{k}^\dagger \right)\!: = \sum_{\mathbf{k}\in \mathrm{BZ}} \omega_k a_\mathbf{k}^\dagger a_\mathbf{k} \tag{3.50}$$

where the operators are ordered such that the annihilation operators appear to the right. By definition, the normally ordered $:H:$ gives zero when acting on the vacuum state.

Eq.(3.49) can also be used to show that the commutator between H and the field operator (3.47) generates the equations of motion:

$$\mathrm{i}\,[H, \Phi] = \partial_t \Phi \tag{3.51}$$

which is of course the Heisenberg equation for the observable Φ. This can be stated in a different way: the operator H generates the translation in time of the field operator. This is a first step towards the relativistic invariance of the theory: time and space translations are part of the Lorentz-Poincaré symmetry group that every relativistic field theory should take into account.

The space translations are generated by the total momentum operator

$$\mathbf{P} = \sum_{\mathbf{k}\in \mathrm{BZ}} \mathbf{k} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}, \qquad \mathrm{i}\,[\mathbf{P}, \Phi] = \nabla \Phi \tag{3.52}$$

Similar operators can be constructed to generate rotations and Lorentz transformations, see the book by Itzykson & Zuber.

We finally note that the following particle number operator commutes with the Hamiltonian:

$$N = \sum_{\mathbf{k}\in \mathrm{BZ}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} \tag{3.53}$$

It is curious to note that this operator is of course positive definite. The problem with the 'negative energy solutions' of the classical theory apparently does not appear in the quantum theory: both total energy and particle number are positive. However, it is not easy to give a local formulation to the particle number (density): to ensure that this is positive as well, one typically needs some spatial smearing.

3.4.3 Field propagator and commutator

To finish the discussion of the free Klein-Gordon theory, let us work out the commutator of the field operator between two space-time points x and y. If $\Phi(x)$ and $\Phi(y)$ are 'independent' observables, this should be zero. Any non-zero result is indicating that the field operator at event x can influence the operator at y: this is of course a check of causality in the relativistic setting. Using $\left[a_{\mathbf{k}},\, a^\dagger_{\mathbf{k}'}\right] = \delta_{\mathbf{k}\mathbf{k}'}$, we get

$$\mathrm{i}\big[\Phi(x),\, \Phi(y)\big] = \sum_{\mathbf{k}\in \mathrm{BZ}} \frac{\mathrm{i}}{2\omega_k V} \left(\mathrm{e}^{-\mathrm{i}k_\mu (x^\mu - y^\mu)} - \mathrm{e}^{\mathrm{i}k_\mu (x^\mu - y^\mu)} \right) \tag{3.54}$$

where the relativistically invariant integration measure d^3k/ω_k appears in the $V \to \infty$ limit (see Exercise 6.2)

$$\mathrm{i}\big[\Phi(x),\, \Phi(y)\big] = \int \frac{\mathrm{d}^3 k}{(2\pi)^3 \omega_k} \sin k_\mu (x^\mu - y^\mu) \equiv D(x-y) \tag{3.55}$$

In Exercise 6.2, you have also shown that the function $D(x)$ only depends on the Minkowski distance $x_\mu x^\mu$. In particular, for $x^0 = 0$, one has $D(0, \mathbf{x}) = 0$ because the function under the integral is odd in $\mathbf{k}$. By Lorentz invariance, this property holds for any space-like separation: we find that indeed, the field operators commute if the two events are not inside each other's light cone.

For time-like separations, one can analyze $D(t, \mathbf{0})$ as a function of t. With the change of variable $k \mapsto \omega_k$, one can show that

$$D(t, \mathbf{0}) = -\frac{m}{8\pi|t|} J_1(mt) \tag{3.56}$$

where J_1 is the first-order Bessel function. The function (3.56) jumps at $t = 0$ from positive to negative values (the size of the jump is $-m^2/8\pi$)[7] and decays smoothly to zero on a time scale $1/m$ with oscillations that have an envelope $\propto t^{-3/2}$. This implies that the commutator is nonzero on the light cone. Nonzero values are found also in the interior of the light cone (in the 'forward' and 'backward' directions) with a width of order $1/m$.

The commutator $D(x - y) = \mathrm{i}\big[\Phi(x), \Phi(y)\big]$ is thus a c-number valued distribution; it is called the 'propagator' of the quantized Klein-Gordon field. This special propagator is not 'causal' in the sense that it propagates the field into the future (then it would be zero on one side of the light cone), but rather contains a superposition of incoming and outgoing spherical waves.

3.5 Particle decay and quantum dissipation

A key fact that must be implemented by quantum field theory is the creation and annihilation of particles. We have already seen that the operators $a^\dagger$ and a with the same name can do this job. But is we want to implement the 'conversion' of particles of one species into another one, we have to specify an interaction between quantum fields. On the level of charged fields coupled to the electromagnetic field, the interaction Hamiltonian can be found from the minimal coupling procedure, but one has to quantize the electromagnetic field as well which comes with some technical difficulties. We discuss here a simpler example: a 'self-interacting Klein-Gordon field', also known as Φ^3-theory.

In the phonon picture, this models the anharmonicity of the crystal lattice. As a consequence, the phonon modes are no longer normal modes of

[7] One can actually show that $\partial_t D(0, \mathbf{x}) = -\delta(\mathbf{x})$.

the system, but mode coupling and mode conversion occurs. In the quasiparticle language: a given phonon is unstable and decays into a pair of phonons.

To describe the decay of particles in quantum field theory, we need two ingredients: • Fermi's Golden Rule, as coming from time-dependent perturbation theory, and • an interaction Hamiltonian that is not just bilinear in the field operators.

3.5.1 Fermi's Golden Rule

This is a key result of time-dependent perturbation theory. See Appendix A for details. The result is the following transition probability per unit time for an initial state $|i\rangle$, summed over all final states $|f\rangle$ allowed by energy conservation:

$$\gamma_{i\to f} = \frac{dw_{i\to f}}{dT} = \frac{2\pi}{\hbar}\sum_f |\langle f|V|i\rangle|^2\,\delta(E_f - E_i) \tag{3.57}$$

Here, E_i and E_f are the initial and final energies, and V is the interaction Hamiltonian.

3.5.2 Interacting bosons

We take here the simplest interaction within a scalar field theory:

$$V = \lambda \int_V \mathrm{d}^3x\,\Phi^3(\mathbf{x}) \tag{3.58}$$

In the phonon picture, this corresponds to a nonlinear term in the vibrations of the lattice. In the field theory, it is called a 'self-interaction'.

What kind of matrix elements involving this V can be nonzero? We shall focus on initial states containing one particle, $|i\rangle = a^\dagger_{\mathbf{p}}|\mathrm{vac}\rangle$. By inserting the mode expansion (3.47) of the field operator, we get for example terms of the form

$$V \propto \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} (\cdots) a^\dagger_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_2} a^\dagger_{\mathbf{k}_3} \tag{3.59}$$

that create three particles. However, since this requires an energy of at least mc^2 for each particle, this process cannot conserve energy. One must change the energy of the initial particle, but this requires an operator sequence of the form $a^\dagger_{\mathbf{k}} a_{\mathbf{k}'}$ to be applied to $|i\rangle$.

Another group of terms is of the form

$$a_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_2} a_{\mathbf{k}_3}$$

where the initial particle is annihilated (if $\mathbf{k}_3 = \mathbf{p}$). The vacuum expectation value of $a_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_2}$ is nonzero if $\mathbf{k}_1 = \mathbf{k}_2$ so that it seems that the initial particle could simply disappear. But again, this process violates energy conservation because $E_i = E_{\mathbf{p}} = (m^2 + \mathbf{p}^2)^{1/2}$, while $E_f = 0$ (zero particles left).

We find a nonzero contribution for the decay into a pair of particles, coming from the combination

$$a^\dagger_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_2} a_{\mathbf{k}_3} \tag{3.60}$$

provided $\mathbf{k}_3 = \mathbf{p}$. If we take as final state $\langle f| = \langle \mathrm{vac}| a_{\mathbf{p}_1} a_{\mathbf{p}_2}$ we find a nonzero matrix element for the terms (3.60) with $\mathbf{k}_1 = \mathbf{p}_1$ and $\mathbf{k}_2 = \mathbf{p}_2$ (or vice versa). The space integral in Eq.(3.58) leads to the momentum conservation rule, $V\delta_{\mathbf{p}_1+\mathbf{p}_2,\mathbf{p}}$, written here for discretized momenta in a finite normalization volume.

We finally integrate over the final momenta $\mathbf{p}_{1,2}$ of the two final particles to get the decay rate for the initial state. After some calculations, this leads to the integral

$$\gamma_{\mathbf{p}} = \pi\lambda^2 \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{\delta(E_1(\mathbf{q}) + E_2(\mathbf{q}) - E_{\mathbf{p}})}{E_1(\mathbf{q}) E_2(\mathbf{q}) E_{\mathbf{p}}} \tag{3.61}$$

where $E_{\mathbf{p}}$ is again the energy of the initial particle. The momentum $\mathbf{q} = \mathbf{p}_1 - \mathbf{p}_2$ is the relative momentum of the particle pair. Its total momentum must be equal to $\mathbf{p}$. Therefore, the energies are

$$E_{1,2}(\mathbf{q})^2 = m^2 + \frac{1}{4}(\mathbf{p} \pm \mathbf{q})^2 \tag{3.62}$$

and the factors $1/E_{\mathbf{p}_i}$ come from the Lorentz-invariant integration measure in three-dimensional momentum space.

There is a threshold energy for the particle decay: since $E_1(\mathbf{q}) + E_2(\mathbf{q}) \geq 2m$, the initial particle must have an energy of at least $E_{\mathbf{p}} \geq 2m$ to decay into this pair. The maximum value of q that can contribute to the integral (3.61) is also easy to find out. An explicit evaluation of the integral is probably possible, but tedious. This kind of integrals is typical for results in elementary particle physics. One is saying that the decay rate is proportional to the 'phase space' available for the products of the decay (given conservation of total energy and momentum). On the other hand, the decay rate is proportional to the squared coupling constant λ^2. This is typical for calculation based on Fermi's Golden Rule (A.34).

3.5.3 Irreversible quantum dynamics

... positive maps, master equations

3.6 Relativistic Dirac field

We would like to illustrate here a key point of quantum field theory: particles with spin $1/2$ (or spin $3/2$, ...) have to be quantized in a different way from spin 0, 1, ...particles. The latter ones (like phonons) are called 'bosons': they can occupy a given field mode in arbitrary numbers $a^\dagger a = 0, 1, 2, \ldots$, as we have seen for phonons. This is forbidden for half-integer spins or 'fermions' where Pauli's exclusion principle holds. There, $a^\dagger a = 0, 1$ are the only allowed occupation numbers for a given mode (this includes the spin quantum number, of course). We shall see that this is related to the occurrence of creation and annihilation operators that are 'anti-commuting'. Our example is the Dirac field, but without the coupling to the electromagnetic field.

3.6.1 Field operator

We follow the quantization scheme that could be called 'correspondence' principle and take the classical energy and momentum density that follow with Noether's theorem from the Dirac Lagrangian. In the energy density integrated over all space, we promote the Dirac field to an operator in such a way that the energy operator generates time translations. Similarly for the momentum operator that generates space translations.

A reminder of Noether's theorem: if a Lagrangian depends on the coordinate $x = (t, \mathbf{x})$ only via the fields Ψ (and their derivatives), the action integral is not changed under a translation of the field arguments (just shift the variables for the integration $\mathrm{d}^4x = \mathrm{d}t\,\mathrm{d}^3x$). For an infinitesimal x-dependent translation by $\delta a^\mu(x)$, we have

$$\delta\Psi(x) = \delta a^\nu(x)\partial_\nu\Psi(x) \tag{3.63}$$

and the derivative of this quantity for $\partial_\mu\delta\Psi$. A calculation leads to

$$0 = \int \mathrm{d}^4x\,(\partial_\mu T^{\mu\nu})\delta a_\nu(x) \tag{3.64}$$

$$T^{\mu\nu} = \frac{\partial\mathcal{L}}{\partial(\partial_\mu\Psi_\alpha)}\partial^\nu\Psi_\alpha(x) - g^{\mu\nu}\mathcal{L} \tag{3.65}$$

The index α is summing over the components of the field, if needed. The quantity $T^{\mu\nu}$ is the energy-momentum tensor of the field theory. It is locally conserved, $\partial_\mu T^{\mu\nu} = 0$, which gives four conserved quantities.

For $\mu, \nu = 0, 0$, one gets the energy density whose integral is the total

energy or Hamiltonian

$$H = \int \mathrm{d}^3x \left\{ \frac{\partial \mathcal{L}}{\partial(\partial_t \Psi_\alpha)} \partial_t \Psi_\alpha(x) - \mathcal{L} \right\} \tag{3.66}$$

we recognize the standard form here, since the first factor contains the momentum conjugate to $\Psi(x)$.

In the Dirac Langrangian,

$$\mathcal{L} = \int \mathrm{d}^3x \left[\frac{\mathrm{i}}{2} \overline{\Psi} \gamma^\mu \partial_\mu \Psi - \frac{\mathrm{i}}{2} \partial_\mu \overline{\Psi} \gamma^\mu \Psi - m \overline{\Psi} \Psi \right], \tag{3.67}$$

the field $\Psi(x)$ and its conjugate $\Psi^\dagger(x) = \overline{\Psi}\gamma^0$ occur. We interpret these as different 'components' of the same field and get a total energy

$$H = \int \mathrm{d}^3x \, \frac{\mathrm{i}}{2} \left(\Psi^\dagger \partial_t \Psi - \partial_t \Psi^\dagger \Psi \right) \tag{3.68}$$

The term $-\mathcal{L}$ does not contribute if we use the Dirac equation, restricting the analysis to fields (operators) whose dynamics satisfies the Dirac equation.[8] We expand the Dirac field into plane waves of particle-like and antiparticle-like character:

$$\Psi(x) = \sum_{\mathbf{k},\sigma} \left[a_{\mathbf{k}\sigma} u_{\mathbf{k}\sigma} \mathrm{e}^{-\mathrm{i}k_\mu x^\mu} + b^\dagger_{\mathbf{k}\sigma} v_{\mathbf{k}\sigma} \mathrm{e}^{\mathrm{i}k_\mu x^\mu} \right] \tag{3.69}$$

where $u_{\mathbf{k}\sigma}$ and $v_{\mathbf{k}\sigma}$ are the spinor-valued amplitudes for a particle- and antiparticle-like plane-wave states with momentum $\mathbf{k}$ and spin quantum number σ. More precisely: these spinors are those one gets if the Dirac solutions for particles at rest (positive or negative energies $\pm m$) are subject to a Lorentz transformation. This explains also the negative sign of the exponential $\mathrm{e}^{\mathrm{i}k_\mu x^\mu}$ in the antiparticle-like term. The operator $a_{\mathbf{k}\sigma}$ annihilates a particle, as we shall see below. The operator $b^\dagger_{\mathbf{k}\sigma}$ creates an anti-particle: we also see below that this choice is the one that ensures that the total energy is positive.

3.6.2 Anticommutators and the Pauli principle

By working out the total energy in terms of this plane wave expansion, we need some orthogonality relations that follow from the Lorentz invariance

[8] In other words, $\mathcal{L} = 0$, for solutions of the equations of motion: this is the technical reason why the standard canonical quantization procedure runs into trouble.

of $\overline{u}_{\mathbf{k}\sigma} v_{\mathbf{k}'\sigma'}$. More details are found in Itzykson & Zuber. The key observation is that the energy (3.68) brings, from the time derivative, the energies $\pm E_k = \pm(m^2 + k^2)^{1/2}$ into the game. The resulting total energy is

$$H = \sum_{\mathbf{k},\sigma} E_k \left[a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} - b_{\mathbf{k}\sigma} b^\dagger_{\mathbf{k}\sigma} \right] \tag{3.70}$$

that we want to interpret as a Hamiltonian. Let us proceed as usual first: the negative sign in front of the anti-particle like number operator $b^\dagger_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma} = b_{\mathbf{k}\sigma} b^\dagger_{\mathbf{k}\sigma} - 1$ is coming from the fact that these modes have 'negative energy'. If we permit that this number operator has arbitrarily large eigenvalues, then the energy (3.70) is getting arbitrary large. This is what we want to avoid in order to get a (dynamically and thermodynamically) stable ground state.

The genial idea to make H positive is the rule

$$b_{\mathbf{k}\sigma} b^\dagger_{\mathbf{k}\sigma} = 1 - b^\dagger_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma} \tag{3.71}$$

so that the number operator $b^\dagger_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma}$ now appears with the opposite sign in Eq.(3.70). We can now identify the vacuum state as usual by $a_{\mathbf{k}\sigma}|\mathrm{vac}\rangle = b_{\mathbf{k}\sigma}|\mathrm{vac}\rangle = 0$. The (infinite) value of the energy in the vacuum state, $-\sum_{\mathbf{k},\sigma} E_k$, is subtracted (this looks like the energy when all modes with negative energy are filled with exactly one particle). After normal ordering, we get the following, nicely looking positive Hamiltonian

$$:H: = \sum_{\mathbf{k},\sigma} E_k \left[a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + b^\dagger_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma} \right]. \tag{3.72}$$

This prescription can be generalized by imposing that the particle and antiparticle creation and annihilation operators are anti-commuting:

$$\delta_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = \left\{ a_{\mathbf{k}\sigma},\, a^\dagger_{\mathbf{k}'\sigma'} \right\} \equiv a_{\mathbf{k}\sigma} a^\dagger_{\mathbf{k}'\sigma'} + a^\dagger_{\mathbf{k}'\sigma'} a_{\mathbf{k}\sigma}, \tag{3.73}$$

similarly for the $b_{\mathbf{k}\sigma'}$, and

$$0 = \left\{ a_{\mathbf{k}\sigma},\, a_{\mathbf{k}'\sigma'} \right\} = \left\{ a_{\mathbf{k}\sigma},\, b^\dagger_{\mathbf{k}'\sigma'} \right\} = \left\{ a_{\mathbf{k}\sigma},\, b_{\mathbf{k}'\sigma'} \right\} \tag{3.74}$$

Note that the relations involving a and a are 'new': we did not have to specify this separately in the boson case. This implies in particular that when one applies a creation (or annihilation) operator twice, one gets nothing:

$$(a^\dagger_{\mathbf{k}\sigma})^2 |\mathrm{vac}\rangle = \frac{1}{2} \left\{ a^\dagger_{\mathbf{k}\sigma},\, a^\dagger_{\mathbf{k}\sigma} \right\} |\mathrm{vac}\rangle = 0 \tag{3.75}$$

It is not possible to create more than one particle in a given mode: this implements the Pauli exclusion principle.

Note, however, that the fermionic (anti-)commutation rules still permit the usual interpretation of the number operator. This comes from the following magic algebra:

$$\left[a_k^\dagger a_k, a_{k'}^\dagger\right] = a_k^\dagger \left\{a_k,\, a_{k'}^\dagger\right\} - \left\{a_k^\dagger,\, a_{k'}^\dagger\right\} a_k = a_k^\dagger \delta_{kk'} \tag{3.76}$$

so that the action of $a_k^\dagger$ increases the particle number $a_k^\dagger a_k$ in mode k by one.

3.6.3 Antiparticles

Similarly, after 'normal ordering', the total number of particles becomes

$$N = \int \mathrm{d}^3x \;:\Psi^\dagger \Psi: = \sum_{\mathbf{k},\sigma} \left[a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} - b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma}\right]. \tag{3.77}$$

This can now be negative or positive! It is funny that in the quantum field theory, this does no longer pose a problem.[9] The negative particle number can be interpreted as the difference between 'particles' and 'anti-particles' or as the total charge (since particles and anti-particles have opposite charges).

To summarize, in the quantization of the Dirac field, one imposes that the total energy be positive (increasing from the vacuum state as particles are created), and this can be done by imposing anti-commutation rules for the mode operators $a_{k\sigma}$ and $a_{k\sigma}^\dagger$. These anti-commutation rules automatically imply the Pauli principle: a given mode for spin 1/2 particles can never be filled by more than one particle.

The filled Fermi sea. We could have formulated the Dirac quantization in terms of the operator $c_{k\sigma} = b_{k\sigma}^\dagger$. In that case, the energy for an anti-particle mode would have scaled like $-E_k c_{k\sigma}^\dagger c_{k\sigma}$. We can re-phrase the preceding construction by saying that • the number operator involved here must have the maximum value 1; • the ground state is given by the 'Fermi sea', a state where all c-modes are filled,

$$|\mathrm{Fermisea}\rangle = \prod_{k\sigma} c_{k\sigma}^\dagger |\mathrm{empty}\rangle;$$

and • Pauli's principle holds, $(c_{k\sigma}^\dagger)^2 = 0$. All these elements are automatically verified by using anti-commutators. In fact, when using anti-commutators,

[9] In fact, the quantum-mechanical probability that must be positive in quantum theory, is 'living' in another space: it is related to the complex probability amplitudes in quantum state superpositions like $\alpha|\mathrm{vac}\rangle + \beta a_k|\mathrm{vac}\rangle$.

annihilation and creation operators can somehow be exchanged: 'create an anti-particle', $b^\dagger$, is like 'destroy a particle of the Fermi sea', c. On the two-dimensional Hilbert space spanned by the states $b^\dagger|\mathrm{vac}\rangle = (1,0)^T$ and $|\mathrm{vac}\rangle = (0,1)^T$, the operators b and $b^\dagger$ are represented by the 'Pauli matrices'

$$b^\dagger \leftrightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad b \leftrightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

whose square is obviously zero.

3.7 Quantum field theory for many-body systems

In this section, we would like to illustrate the connection between the quantum field theory formulated up to now and the usual non-relativistic many-body quantum mechanics. You are probably familiar with the fact that for systems of indistinguishable particles, quantum statistics comes into play: the wave function $\psi(\mathbf{x}_1, \ldots \mathbf{x}_N)$ must be symmetric or anti-symmetric under particle exchange. For example,

$$\text{bosons/fermions: } \psi(\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3 \ldots \mathbf{x}_N) = \pm\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \ldots \mathbf{x}_N) \tag{3.78}$$

More generally the sign $\varepsilon(\pi)$ of the permutation π of particle coordinates occurs in $\psi(\mathbf{x}_{\pi 1}, \ldots \mathbf{x}_{\pi N})$ for fermions, while the many-boson wave function is totally symmetric under permutations.

3.7.1 N-particle sectors in Fock space

What is the connection to the field operator? The general picture is the following: the field operator $\Psi(\mathbf{x})$ connects parts of the Hilbert space that differ by one in the total particle number (it is a combination of operators that create or annihilate one particle). However, these 'sectors' typically evolve indepedently since the particle number N commutes with the Hamiltonian. In a simple non-relativistic theory, one has

$$H = \sum_k E_k a_k^\dagger a_k, \qquad N = \sum_k a_k^\dagger a_k. \tag{3.79}$$

N commutes with H because one requires an energy mc^2 to create an extra particle. The 'one-particle sector' $\mathcal{H}_1$ is spanned by the states $a_k^\dagger|\mathrm{vac}\rangle$. One can thus ask: what is the 'wave function' of these states? If the k label plane wave states, then $a_k^\dagger|\mathrm{vac}\rangle$ is an eigenstate of the momentum operator $\hat{P}$ with eigenvalue k:

$$\hat{P} = \sum_k k a_k^\dagger a_k \tag{3.80}$$

In the non-relativistic limit, it is useful to separate the field operator into positive and negative frequency components Ψ and $\Psi^\dagger$. The positive frequency part contains only annihilation operators:[10]

$$\Psi(\mathbf{x},t) = \sum_k a_k(t)\phi_k(\mathbf{x}), \qquad \Psi^\dagger(\mathbf{x},t) = [\Psi(\mathbf{x},t)]^\dagger \tag{3.81}$$

with orthonormal mode functions $\phi_k(\mathbf{x})$.

One-particle states.

The field operator $\Psi^\dagger(\mathbf{x}')$, when acting on the vacuum state, produces a quantum state in the one-particle sector $\mathcal{H}_1$. Its probability amplitude in the momentum representation is given by (up to a normalization)

$$\tilde{\psi}(k;\mathbf{x}') = \langle \mathrm{vac}|a_k\Psi^\dagger(\mathbf{x}')|\mathrm{vac}\rangle \tag{3.82}$$

With the mode expansion (3.81), adding (subtracting) the vanishing average $\langle \mathrm{vac}|\Psi^\dagger(\mathbf{x}')a_k|\mathrm{vac}\rangle$ and using the (anti)-commutation rules for the a_k's, we get

$$\tilde{\psi}(k;\mathbf{x}') = \phi_k^*(\mathbf{x}') \tag{3.83}$$

In the position representation, we thus have a 'wave function'

$$\psi(\mathbf{x};\mathbf{x}') = \sum_k \phi_k^*(\mathbf{x}')\phi_k(\mathbf{x}) = \delta(\mathbf{x}-\mathbf{x}') \tag{3.84}$$

where we used the completeness relation of the mode functions $\phi_k(\mathbf{x})$. Hence, $\Psi^\dagger(\mathbf{x}')|\mathrm{vac}\rangle$ is a state localized at the position $\mathbf{x}'$, or in other words:

> the field operator $\Psi^\dagger(\mathbf{x}')$ [$\Psi(\mathbf{x}')$] creates [annihilates] a particle at the position $\mathbf{x}'$.

We can interpret the same calculation in terms of the wave function (in the usual sense, i.e., in the position representation) of the states creates by $a_k^\dagger$. Projecting onto the position eigenstate $\Psi^\dagger(\mathbf{x})|\mathrm{vac}\rangle$, we have

$$\langle \mathrm{vac}|\Psi(\mathbf{x})a_k^\dagger|\mathrm{vac}\rangle = \phi_k(\mathbf{x}) \tag{3.85}$$

Hence the plane wave mode function is also the quantum-mechanical wave function for the one-particle state associated with the mode k.

[10] In the Klein-Gordon theory, the separation into positive and negative frequencies is natural. In the case of the relativistic Dirac field $\Psi_D(x)$, one can write $\Psi_D(x) \approx \mathrm{e}^{-\mathrm{i}mc^2t/\hbar}\Psi(x)$ and make $\Psi(x)$ slowly varying in time by averaging it over a time scale of order $\hbar/mc^2$. This makes the anti-particle contribution disappear that evolves at negative frequencies.

Two-particle states.

Two-particle states are generated by the basis states $a_k^\dagger a_{k'}^\dagger|\text{vac}\rangle$ with $k \neq k'$ in the Fermion case. To compute their wave function $\psi(\mathbf{x}_1, \mathbf{x}_2)$, we project onto the two-particle position state $\Psi^\dagger(\mathbf{x}_2)\Psi^\dagger(\mathbf{x}_1)|\text{vac}\rangle$:

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \langle \text{vac}|\Psi(\mathbf{x}_1)\Psi(\mathbf{x}_2)a_k^\dagger a_{k'}^\dagger|\text{vac}\rangle \tag{3.86}$$

By a calculation similar to the previous one, we shift the annihilation operators in $\Psi(\mathbf{x}_1)$ and $\Psi(\mathbf{x}_2)$ through $a_k^\dagger$ and $a_{k'}^\dagger$ and use the (anti)commutation rules. The result is

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \phi_{k'}(\mathbf{x}_1)\phi_k(\mathbf{x}_2) \pm \phi_k(\mathbf{x}_1)\phi_{k'}(\mathbf{x}_2) \tag{3.87}$$

which is even (odd) under the exchange of the coordinates $\mathbf{x}_1$ and $\mathbf{x}_2$, depending on Bose or Fermi statistics. We could have anticipated this result: since the operators $a_k^\dagger$ and $a_{k'}^\dagger$ (anti)commute, the two-particle state $a_k^\dagger a_{k'}^\dagger|\text{vac}\rangle$ must be even (odd) in the quantum numbers k and k'.

Similarly, one can show that the state $a_{k_1}^\dagger \dots a_{k_N}^\dagger|\text{vac}\rangle$ is totally (anti)symmetric in the quantum numbers $k_1, \dots k_N$, and its wave function $\psi(\mathbf{x}_1, \dots \mathbf{x}_N)$ behaves similarly.

Fermion creators and annihilators

Operators are acting in unusual way on Fock states. See Dawydow's book on quantum mechanics, § 86.

3.7.2 Many-body Hamiltonian

To conclude, we write down the link between the usual formulation of a quantum many-body theory for particles that interact via a potential $V(\mathbf{r})$ and the quantum field theory (or 'second quantized') language. The many-body Hamiltonian is, for N indistinguishable particles

$$H = \sum_{\alpha=1}^{N} \left(\frac{\mathbf{p}_\alpha^2}{2m} + W(\mathbf{x}_\alpha) \right) + \frac{1}{2} \sum_{\alpha \neq \beta} V(\mathbf{x}_\alpha - \mathbf{x}_\beta) \tag{3.88}$$

where $W(\mathbf{x})$ is an 'external potential' that is the same for all particles. Of course, the momentum operator is $\mathbf{p}_\alpha = -\mathrm{i}\hbar\nabla_\alpha$, the derivative with respect to the α'th coordinate. The particle density, for example, is given by the operator

$$n(\mathbf{x}) = \sum_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha) \tag{3.89}$$

In second quantization, the particle density becomes

$$n(\mathbf{x}) = \Psi^\dagger(\mathbf{x})\Psi(\mathbf{x}) \tag{3.90}$$

while the Hamiltonian is (in normally ordered form)

$$\begin{aligned} H &= \int \mathrm{d}^3x \left(\frac{\hbar^2}{2m} \nabla\Psi^\dagger \cdot \nabla\Psi + \Psi^\dagger(\mathbf{x}) W(\mathbf{x}) \Psi(\mathbf{x}) \right) \\ &\quad + \frac{1}{2} \int \mathrm{d}^3x \mathrm{d}^3x' \Psi^\dagger(\mathbf{x}) \Psi^\dagger(\mathbf{x}') V(\mathbf{x}-\mathbf{x}') \Psi(\mathbf{x}') \Psi(\mathbf{x}). \end{aligned} \tag{3.91}$$

This formulation is the starting point for the discussion of several phenomena in physics: electron waves in condensed matter and superconductivity, liquid Helium and superfluidity, atomic matter waves at low temperatures and Bose-Einstein condensation. Generally speaking, the temperature of the system is a key parameter here, and one is looking for equilibrium correlation functions of the form

$$\langle \Psi^\dagger(\mathbf{x},t)\Psi(\mathbf{x}',t')\rangle_T, \qquad \langle n(\mathbf{x},t)n(\mathbf{x}',t')\rangle_T \tag{3.92}$$

These functions can actually be measured by interference or scattering experiments.

In some of these applications, one works in a statistical ensemble where the particle number N is not fixed because the system is in contact with a 'particle reservoir'. This can be a good approximation even in the case where one knows that N is conserved, because in the thermodynamic limit $N \to \infty$, the fluctuations in the particle number are getting small.[11] The ground state of the system in this ensemble is found by minimizing the so-called 'grand-canonical Hamiltonian'

$$K = H - \mu N \tag{3.93}$$

where μ is called the 'chemical potential'. Its value is fixed by the requirement that the average particle number coincides with a given number $\bar{N}$:

$$\bar{N} = \frac{\partial}{\beta \partial \mu} \log \mathrm{tr}\, \exp(-\beta K) \tag{3.94}$$

where the trace gives the partition function (*Zustandssumme*) in this ensemble.

In the following, we try to avoid the grand-canonical ensemble and work with a system in an eigenstate to the particle number operator N.

[11] The Bose-Einstein condensation of an ideal gas is an exception and shows a peculiar scaling with N in this respect, see M. Wilkens and C. Weiss, *J. mod. Optics* **44** (1997) 1801.

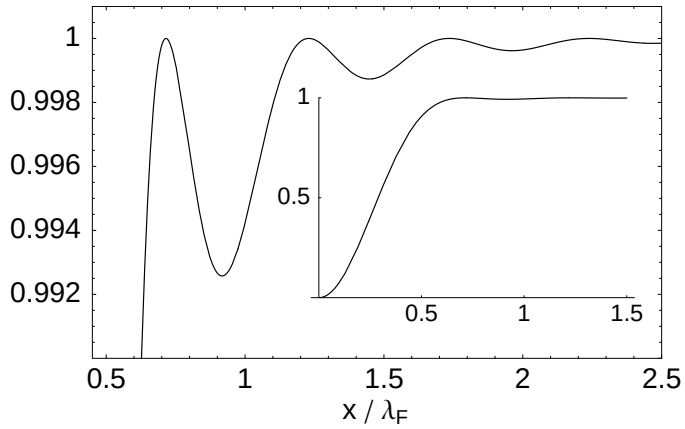

Figure 3.4: Average pair density $\langle n_2(\mathbf{x}-\mathbf{y})\rangle$ in a homogeneous, ideal Fermi gas, vs. distance $x = |\mathbf{x}-\mathbf{y}|$. Inset: short distance $x \sim \lambda_F = 2\pi/k_F$.

3.8 Example: density correlations in a Fermi gas

Goal: Friedel oscillations in the density-density correlations, even without interactions.

Basic quantities:

density operator $n(\mathbf{x}) = \psi^\dagger(\mathbf{x})\psi(\mathbf{x})$

pair density operator $n_2(\mathbf{x},\mathbf{y}) = \psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{y})\psi(\mathbf{y})\psi(\mathbf{x})$

Expansion of field operator in plane waves in "quantization volume" V.

Fermi sea: "ground state" with the constraint that N particles are present in V (density N/V). Single-particle states filled up until $|\mathbf{k}| \le k_F$ with Fermi wavenumber k_F and Fermi energy.

average value of density in the ground state and E_F

expectation value of density correlations: need expectation value $\langle a^\dagger_{\mathbf{p}} a^\dagger_{\mathbf{q}} a_{\mathbf{r}} a_{\mathbf{s}}\rangle$. Work out with fermionic anticommutators.

Result for spin-polarized Fermi gas:

$$\langle n_2(\mathbf{x},\mathbf{y})\rangle = \langle n\rangle^2 \left[1 - \left(\frac{3(\sin k_F x - k_F x \cos k_F x)}{(k_F x)^3}\right)^2\right] \tag{3.95}$$

where $x = |\mathbf{x}-\mathbf{y}|$. See plot 3.4.

Comment: 'repulsion' just due to Pauli principle, even without any physical interaction. Other interpretation of Friedel oscillations: typical two particle wave function (in usual two-body quantum mechanics language)

$$\psi_{\mathbf{k},\mathbf{k}'}(\mathbf{x},\mathbf{y}) \propto \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{y}} - \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{x}} \tag{3.96}$$

with a pair density $n_2(\mathbf{x},\mathbf{y}) = |\psi_{\mathbf{k},\mathbf{k}'}(\mathbf{x},\mathbf{y})|^2$. To be averaged over Fermi-Dirac distribution for momenta $\mathbf{k}$, $\mathbf{k}'$.

3.9 Example: superconductivity

Example of interactions that change the character of the excitation spectrum.

3.9.1 Ginzburg-Landau wave function

3.9.2 Bardeen-Cooper-Schrieffer theory

Basic properties: energies of lowest excitation. For each particle, count energies from Fermi energy E_F, i.e. shift energy by NE_F.

Ideal Fermi gas. Single-particle energy

$$H^{(1)} = \sum_{\mathbf{k},s} \left(\hbar^2\mathbf{k}^2/2m - E_F\right) a^\dagger_{\mathbf{k},s} a_{\mathbf{k},s}$$

'particle-like' excitation with energy $E_\mathbf{k} = \hbar^2\mathbf{k}^2/2m - E_F$ for $|\mathbf{k}| \geq k_F$. Low-energy limit:

$$E_\mathbf{k} \approx \hbar v_F \left(|\mathbf{k}| - k_F\right)$$

with $v_F = \hbar k_F/m$. Similar to sound waves.

'hole-like' excitation: remove electron from Fermi sea. Hence $|\mathbf{k}| \leq k_F$ and $\hbar^2\mathbf{k}^2/2m - E_F < 0$. Write in 'hole representation'

$$\begin{aligned} a_{\mathbf{k},s} &= B^\dagger_{-\mathbf{k},-s}, \qquad a^\dagger_{\mathbf{k},s} a_{\mathbf{k},s} = 1 - B^\dagger_{-\mathbf{k},-s} B_{-\mathbf{k},-s} \\ a^\dagger_{\mathbf{k},s} &= B_{-\mathbf{k},-s} \end{aligned}$$

Hence energy takes the form

$$\begin{aligned} H^{(1)}(\text{holes}) &= \sum_{s,\mathbf{k}\in\text{FS}} \left(\hbar^2\mathbf{k}^2/2m - E_F\right) \left(1 - B^\dagger_{-\mathbf{k},-s} B_{-\mathbf{k},-s}\right) \\ &= E_\text{FS} + \sum_{s,\mathbf{k}\in\text{FS}} \left|\hbar^2\mathbf{k}^2/2m - E_F\right| B^\dagger_{\mathbf{k},s} B_{\mathbf{k},s} \end{aligned} \tag{3.97}$$

with E_FS the energy of the Fermi sea (shifted by NE_F).

The total energy can thus be written in terms of 'occupation numbers' $a^\dagger_{\mathbf{k},s} a_{\mathbf{k},s}$ (above Fermi level) and $B^\dagger_{\mathbf{k},s} B_{\mathbf{k},s}$ (below Fermi level) and positive excitation energies

$$|\varepsilon(\mathbf{k})| = \left|\hbar^2\mathbf{k}^2/2m - E_F\right| \approx \hbar v_F \left||\mathbf{k}| - k_F\right|$$

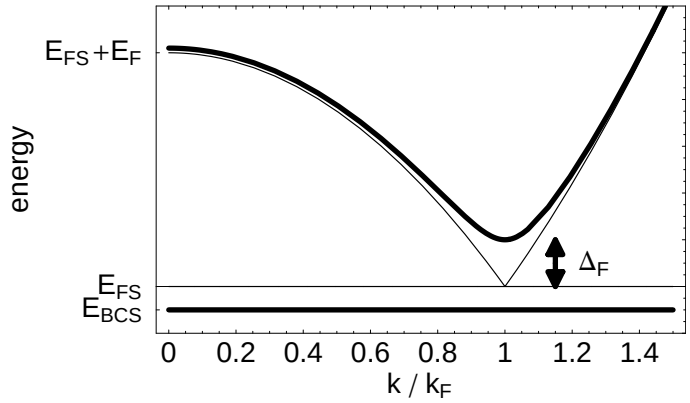

Figure 3.5: Spectrum of elementary excitations. Thin line: ideal Fermi gas. Thick line: with attractive interactions, leading to an energy gap. $E_{\rm FS}$: energy of the (noninteracting) Fermi sea. E_F: Fermi energy. $E_{\rm BCS}$: energy of the (interacting) ground state of the BCS Hamiltonian. k_F: Fermi wavevector.

last approximation valid near the Fermi level.

Plot of single particle excitation spectrum, Fig. 3.5.

With (attractive) interactions. Plot of excitation spectrum: thick lines in Fig.3.5. Ground state shifted down from $E_{\rm FS}$. Single-excitation spectrum with gap $> \Delta_{\mathbf{k}} \geq \Delta_F$ given by Hamiltonian

$$H^{(BCS)} = E_{\rm BCS} + \sum_{\mathbf{k}} \sqrt{\varepsilon^2(\mathbf{k}) + \Delta_{\mathbf{k}}^2} \left(A_{\mathbf{k}}^\dagger A_{\mathbf{k}} + B_{\mathbf{k}}^\dagger B_{\mathbf{k}} \right) \tag{3.98}$$

where $\Delta_{\mathbf{k}}$ is the 'gap function'. We call this the Bardeen–Cooper–Schrieffer (BCS) Hamiltonian who worked out a microscopic theory of superconductivity in 1956.

The operators $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ create 'Cooper pairs': superposition of electron with momentum $\mathbf{k}$ and missing electron at momentum $-\mathbf{k}$ (both quasiparticles have the same net momentum) relative to the Fermi sea. One can build states from these pairs that carry a net current:

electron current: $e\frac{\hbar\mathbf{k}}{m} \times$ density

hole current: $(-e)\frac{\hbar(-\mathbf{k})}{m} \times$ density

equilibrium state with a net current: Fermi sphere centered around mean momentum $m\mathbf{v}_D$, say. Then no excitations can be created by scattering from impurities (who conserve energy) and the 'displaced Fermi sphere' remains a stable ground state.

Require that the change in energy due to the 'moving Fermi sea', $(\hbar\mathbf{k} - m\mathbf{v}_D)^2/2m - (\hbar\mathbf{k})^2/2m \approx -\hbar\mathbf{k}\cdot\mathbf{v}_D$, is small enough compared to the gap. Leads to a condition for the drift velocity since $|\mathbf{k}| \le k_F$: $\hbar k_F v_D < \Delta_F$

Microscopic origin of electron-electron interaction: coupling of electron density to (positive) density of background lattice that is modulated when phonons are present. Superconductivity occurs when this interaction is sufficiently strong, hence for materials that in the normally conducting state are fairly bad conductors.

Calculation of excitation spectrum. Consider an interaction energy that is independent of the particle spin. Then the energy $W(\mathbf{x}-\mathbf{y})$ must be weighted with the total densities $\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x}) = \sum_s \psi_s^\dagger(\mathbf{x})\psi_s(\mathbf{x})$ and $\sum_s \psi_s^\dagger(\mathbf{y})\psi_s(\mathbf{y})$. We get

$$W = \frac{1}{2}\sum_{s,s'}\int \mathrm{d}x\,\mathrm{d}y\,\psi_s^\dagger(\mathbf{x})\psi_{s'}^\dagger(\mathbf{y})W(\mathbf{x}-\mathbf{y})\psi_{s'}(\mathbf{y})\psi_s(\mathbf{x}) \tag{3.99}$$

$$= \frac{1}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{s,s'} a_{\mathbf{k}',s}^\dagger a_{\mathbf{q}-\mathbf{k}',s'}^\dagger \tilde{W}(\mathbf{k}'-\mathbf{k})a_{\mathbf{q}-\mathbf{k},s'}a_{\mathbf{k},s} \tag{3.100}$$

with Fourier transform of potential $\tilde{W}(\mathbf{k}'-\mathbf{k})$.

Model calculation with following simplifications:
The potential $W(\mathbf{x}-\mathbf{y})$ is short range so that it is only effective within the "Friedel–Pauli hole". Hence we need different spin states $s' = -s \neq s$ otherwise the Pauli principle suppresses the interaction.
Consider only states near the Fermi energy, $|\mathbf{k}| \approx k_F$ with $\mathbf{q}-\mathbf{k} \approx -\mathbf{k}$ and $\mathbf{q}-\mathbf{k}' \approx -\mathbf{k}'$ (or: keep only $\mathbf{q}=\mathbf{0}$). These states have the same energy.

With these simplifications, Hamilton operator

$$H = \sum_{\mathbf{k},s}\varepsilon(\mathbf{k})a_{\mathbf{k},s}^\dagger a_{\mathbf{k},s} - \frac{1}{2V}\sum_{\mathbf{k},\mathbf{k}'}\tilde{W}(\mathbf{k}'-\mathbf{k})\sum_s a_{\mathbf{k}',s}^\dagger a_{-\mathbf{k}',-s}^\dagger a_{-\mathbf{k},-s}a_{\mathbf{k},s}$$

Sign of interaction is redefined: positive $\tilde{W}(\mathbf{k}'-\mathbf{k})$ now means attraction. (Sum over spin variable s is trivial, gives a factor 2. Index s replaced by $\uparrow$ in the following or suppressed.)

Key trick to diagonalize this Hamiltonian approximately: "Bogoliubov transformation" (attention: do not confuse v_k with a velocity.)

$$a_{\mathbf{k}\uparrow} = u_k A_k + v_k B_k^\dagger \tag{3.101}$$

$$a_{-\mathbf{k}\downarrow} = u_k B_k^\dagger - v_k A_k \tag{3.102}$$

with new fermionic operators A_k and B_k. (Anti)commutation relations are preserved provided $u_k^2 + v_k^2 = 1$. Assume that u_k, v_k real, and even in k.

Key assumption: $A^\dagger$ and $B^\dagger$ create "quasiparticles" and the ground state and its low-energy excitations are such that the quasiparticle numbers $A^\dagger A$ and $B^\dagger B$ are small. Analogy to hole representation where $a^\dagger a \approx 1$, but $1 - a^\dagger a = B^\dagger B \ll 1$. In fact, the Bogoliubov transformation is a generalization of the hole representation.

Express Hamilton operator in these variables, use anticommutation relations to bring operators in normal order, and get

$$\begin{aligned} H &= \sum_{\mathbf{k}} \left[2\varepsilon(\mathbf{k})v_k^2 - u_k v_k \Delta_{\mathbf{k}}\right] && (3.103)\\ &\quad + \sum_{\mathbf{k}} \left[\varepsilon(\mathbf{k})(u_k^2 - v_k^2) + 2\Delta_{\mathbf{k}} u_k v_k\right] (A_k^\dagger A_k + B_k^\dagger B_k) && (3.104)\\ &\quad + \sum_{\mathbf{k}} \left[2\varepsilon(\mathbf{k})u_k v_k - \Delta_{\mathbf{k}}(u_k^2 - v_k^2)\right] (B_k^\dagger A_k^\dagger + A_k B_k) && (3.105)\\ &\quad + \text{4th order terms} \\ \text{where } \Delta_{\mathbf{k}} &= \frac{1}{V}\sum_{\mathbf{k}'} \tilde{W}(\mathbf{k}' - \mathbf{k}) u_{k'} v_{k'} && (3.106) \end{aligned}$$

The '4th order terms' not explicitly written here are proportional to $A^\dagger A\, B^\dagger B$ or other combination of four fermionic operators. We neglect them in the following.

To proceed, we choose the functions u_k, v_k such that the expression (3.105) with the non-normally ordered operator products AB, $B^\dagger A^\dagger$ vanishes. This is achieved with

$$u_k^2 = \frac{1}{2}\left[1 + \frac{\varepsilon(\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k}) + \Delta_{\mathbf{k}}^2}}\right], \qquad v_k^2 = \frac{1}{2}\left[1 - \frac{\varepsilon(\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k}) + \Delta_{\mathbf{k}}^2}}\right] \tag{3.107}$$

Putting this solution into expression (3.104), we find the following normal mode frequencies for the operators $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$:

$$\varepsilon(\mathbf{k})(u_k^2 - v_k^2) + 2\Delta_{\mathbf{k}} u_k v_k = E(\mathbf{k}) \equiv \sqrt{\varepsilon^2(\mathbf{k}) + \Delta_{\mathbf{k}}^2}$$

that appears in the Hamiltonian together with the number operators $A_k^\dagger A_k + B_k^\dagger B_k$. We have thus found the part (3.98) of the Hamiltonian. The ground state energy is given by the first line (3.103) and can be re-written in the form

$$E_{\mathrm{BCS}} = \sum_{\mathbf{k}} \frac{\varepsilon(\mathbf{k})[E(\mathbf{k}) - \varepsilon(\mathbf{k})] - \frac{1}{2}\Delta_{\mathbf{k}}^2}{E(\mathbf{k})}$$

For large $\Delta \gg \varepsilon$, is it easy to see that this expression is negative. This is also true for small Δ, as is found by expanding the square root. Hence, the

interactions lead to a lowering of the collective ground state of the system. As explained above, the single (quasi)particle excitations start at a minimum energy $\min E(\mathbf{k}) = E(k_F) = |\Delta(k_F)|$ above the ground state. This is called a 'gap' in the spectrum.

So far, everything can be expressed in terms of the 'gap function' $\Delta_{\mathbf{k}}$. Putting the solutions for the Bogoliubov amplitudes into Eq.(3.106), we find the integral equation

$$\Delta_{\mathbf{k}} = \frac{1}{2V}\sum_{\mathbf{k}'} \frac{\Delta'_{\mathbf{k}}\tilde{W}(\mathbf{k}'-\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k}')+\Delta^2_{\mathbf{k}'}}} = \int \frac{\mathrm{d}^3k'}{2(2\pi)^3} \frac{\Delta'_{\mathbf{k}}\tilde{W}(\mathbf{k}'-\mathbf{k})}{\sqrt{\varepsilon^2(\mathbf{k}')+\Delta^2_{\mathbf{k}'}}} \tag{3.108}$$

To solve it, we assume that all relevant $\mathbf{k}$-values are confined to the "Fermi surface", i.e., $|\mathbf{k}| \approx k_F$ and that $\Delta_{\mathbf{k}} = \Delta_F$ is constant there. In addition, we replace $\tilde{W}(\mathbf{k}'-\mathbf{k})$ by a constant, $\tilde{W}_0$. This can be justified by recalling that the potential was assumed to be short-ranged on the scale $\lambda_F = 1/k_F$ of the Friedel oscillations. Hence, its Fourier transform has a support much larger than k_F and can be replaced by its lowest order expansion around $\mathbf{k}'-\mathbf{k} = \mathbf{0}$ for values of $\mathbf{k}'-\mathbf{k}$ with a maximum magnitude of $2k_F$. We also expand

$$\varepsilon(\mathbf{k}') \approx \hbar v_F(k'-k_F)$$

and get

$$1 = \frac{\tilde{W}_0 k_F^2}{(2\pi)^2}\int \frac{\mathrm{d}k'}{\sqrt{(\hbar v_F)^2(k'-k_F)^2+\Delta_F^2}} \tag{3.109}$$

We perform the integral (it gives an arsinh function) with the limits $k' = k_F - q \ldots k_F + q$ to achieve convergence, solve for Δ_F and find

$$\Delta_F = \frac{\hbar v_F q}{\sinh(D/2\tilde{W}_0)}, \qquad D = \frac{2\pi^2\hbar v_F}{k_F^2} = \frac{2\pi^2\hbar^2}{mk_F} \tag{3.110}$$

This result has the interesting property that it is not analytical in the limit $\tilde{W}_0 \to 0$ (one is hitting the essential singularity of the exponential function at infinity; Δ_F goes to zero faster than any power of $\tilde{W}_0$). This is why it is often argued that the Bogoliubov spectrum cannot be found with a perturbation expansion in the interaction strength (this necessarily involves a power series in W).

3.9.3 Coupling to a boson field: effective interactions

Examples: Electron-phonon coupling, leading to an attraction between electrons of opposite spin (Cooper pair formation in superconductivity).

Interactions between electric point charges, due to the coupling to the quantized electromagnetic field.

Interactions between charges in a plasma. The re-arrangement of the other charges gives rise to "screening" and a reduced interaction at large distance.

Interactions between nucleons (neutrons and protons), due to the coupling to the 'pion field'. The pion has a mass, and therefore the interaction has a finite range.

The weak interaction (between quarks and leptons), via a coupling to the 'vector bosons' $W^{\pm}$ and Z_0. Again, an interaction of finite range because the $W^{\pm}$ and Z_0 are massive.

Effective interaction via coupling to a boson field

Simple model (cheating a little bit) to describe the coupling between particles that arises by exciting 'virtual' bosons. This mechanism is also operating to create the Coulomb interaction between charges (photons are created virtually) or the other interactions mentioned above.

Hamiltonian with bosonic operators $a_{\mathbf{q}}$, $a_{\mathbf{q}}^{\dagger}$ and linear interaction:

$$H = \sum_{\mathbf{q}} \omega_q a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} - \sum_{\mathbf{q}} \left(D_{\mathbf{q}} n_{-\mathbf{q}} a_{\mathbf{q}} + \text{h.c.} \right) + H_{\text{F}} \tag{3.111}$$

H_{F} describes the 'rest of the world'.

Justification for this coupling: operators $a_{\mathbf{q}}$, $a_{\mathbf{q}}^{\dagger}$ involved in electric potential $\varphi(\mathbf{x})$. Interaction energy is proportional to $e\varphi(\mathbf{x})n(\mathbf{x})$ with the particle density $n(\mathbf{x})$. Passing to Fourier transform gives Eq.(3.113) with $n_{-\mathbf{q}}$ the Fourier transform of $n(\mathbf{x})$.

Try to get rid of the terms linear in $a_{\mathbf{q}}$ with the following transformation:

$$a_{\mathbf{q}} \mapsto \alpha_{\mathbf{q}} + a_{\mathbf{q}} \tag{3.112}$$

For a more general transformation in the boson case, see the section on Bose-Einstein condensation. With this shift, one preserves the bosonic commutation relations (impossible for anticommutators!), provided $\alpha_{\mathbf{q}}$ commutes with $a_{\mathbf{q}}$, $a_{\mathbf{q}}^{\dagger}$.

We get

$$H = \ldots \tag{3.113}$$

Appendix A

Zeitabhängige Störungstheorie

Problemstellung

Gegeben sei ein Hamiltonoperator

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t) \tag{A.1}$$

wobei die Zeitentwicklung unter $\hat{H}_0$ bekannt sei. Zum Zeitpunkt t_0 sei das System im Eigenzustand $|a\rangle$ von $\hat{H}_0$ präpariert. Gesucht ist die Wahrscheinlichkeit, das System zum Zeitpunkt t im Eigenzustand $|b\rangle$ zu finden:

$$w_{ab}(t) = |\langle b|U(t,t_0)|a\rangle|^2 . \tag{A.2}$$

Hier ist $U(t,t_0)$ der Zeitentwicklungsoperator zum Hamiltonoperator (A.1). Dieser unitäre Operator ist schwieriger auszurechnen als der für das ungestörte System, und wir werden ihn als Potenzreihe im Potential $\hat{V}(t)$ suchen.

Beispiel. Für ein Atom im Lichtfeld etwa ist $\hat{H}_0$ der Hamiltonoperator des Atoms und $\hat{V}(t) = -\hat{\mathbf{d}} \cdot \mathbf{E}(t)$ die elektrische Dipol-Wechselwirkung. Dabei ist $\hat{\mathbf{d}} = -e\hat{\mathbf{q}}$ der elektrische Dipoloperator und $\mathbf{E}(t)$ die elektrische Feldstärke des Lichts am Ort des Atoms.

Vorarbeiten

Wiederholung: Eigenschaften des Zeitentwicklungsoperators. Bewegungsgleichung (= Schrödingergleichung)

$$i\hbar \frac{\partial}{\partial t} U(t,t_0) = \hat{H}(t)\, U(t,t_0) \tag{A.3}$$

Anfangsbedingung

$$U(t_0, t_0) = \mathbf{1} \tag{A.4}$$

Differentialgleichung und Anfangsbedingung lassen sich kombinieren in Integralgleichung

$$U(t, t_0) = \mathbf{1} + \frac{1}{i\hbar} \int_{t_0}^{t} d\tau \, \hat{H}(\tau) U(\tau, t_0) \tag{A.5}$$

Beweis: differenzieren; $t = t_0$ einsetzen.

Schwierigkeit: Gl.(A.5) ist eine Integralgleichung, in der $U(t, t_0)$ auf beiden Seiten auftritt.

Wechselwirkungsbild. Idee: zwar können wir den Zeitentwicklungsoperator zu $\hat{H}(t)$ nicht bestimmen, wohl aber den zu $\hat{H}_0$:

$$U_0(t, t_0) = \exp\left(-i\hat{H}_0(t - t_0)/\hbar\right) \tag{A.6}$$

Seine Wirkung in der Energiedarstellung $|a\rangle, |b\rangle, \ldots |m\rangle, \ldots$ ist diagonal:

$$U_0(t, t_0)|m\rangle = e^{-iE_m(t-t_0)/\hbar}|m\rangle \tag{A.7}$$

Wir definieren einen neuen Zustand $|\tilde{\psi}(t)\rangle$ durch folgende Vereinbarung

$$|\psi(t)\rangle = U_0(t, t_0)|\tilde{\psi}(t)\rangle \tag{A.8}$$

Wozu ist das gut? Aus der Schrödingergleichung kann man folgende Bewegungsgleichung für $|\tilde{\psi}(t)\rangle$ ausrechnen

$$i\hbar \frac{\partial}{\partial t}|\tilde{\psi}(t)\rangle = \tilde{V}(t)|\tilde{\psi}(t)\rangle \tag{A.9}$$

wobei

$$\tilde{V}(t) = U_0^{\dagger}(t, t_0) V(t) U_0(t, t_0) \tag{A.10}$$

Vorteil von Gl.(A.9): die Zeitentwicklung hängt nur noch vom Wechselwirkungsoperator ab.

Wichtiger **Begriff:** mit Hilfe der unitären Transformation (A.8) begibt man sich ins **Wechselwirkungsbild**.

von Neumann-Reihe. Zeitentwicklungsoperator zur Bewegungsgleichung (A.9):

$$|\tilde{\psi}(t)\rangle = U_I(t, t_0)|\tilde{\psi}(t_0)\rangle \tag{A.11}$$

Anfangsbedingung wie vorher. Damit Integralgleichung:

$$U_I(t,t_0) = \mathbf{1} + \frac{1}{i\hbar}\int_{t_0}^{t} d\tau\, \tilde{V}(\tau) U_I(\tau,t_0) \tag{A.12}$$

Wir sind immer noch nicht viel weiter, wenn wir nicht diese Gleichung lösen. Wir bekommen aber eine Potenzreihenentwicklung (die "von Neumann-Reihe"), wenn wir (A.12) iterieren, d.h. auf der rechten Seite die linke Seite einsetzen. Man erhält damit:

$$\begin{aligned}
U_I(t,t_0) &= \sum_{n=0}^{\infty} U_I^{(n)}(t,t_0) && \text{(A.13)}\\
U_I^{(0)}(t,t_0) &= \mathbf{1} && \text{(A.14)}\\
U_I^{(1)}(t,t_0) &= \frac{1}{i\hbar}\int_{t_0}^{t} d\tau\, \tilde{V}(\tau) && \text{(A.15)}\\
U_I^{(2)}(t,t_0) &= -\frac{1}{\hbar^2}\int_{t_0}^{t} \underset{\tau_1>\tau_2}{d\tau_1 d\tau_2}\; \tilde{V}(\tau_1)\tilde{V}(\tau_2) && \text{(A.16)}\\
&\ldots
\end{aligned}$$

Vornehm kann man diese Reihe auch als "zeitgeordnete Exponentialfunktion" schreiben:

$$U_I(t,t_0) = \mathcal{T}\exp\left(\frac{1}{i\hbar}\int_{t_0}^{t} d\tau\, \tilde{V}(\tau)\right) \tag{A.17}$$

wobei $\mathcal{T}$ den (Super-)Operator der Zeitordnung bedeutet: in der Entwicklung des nachfolgende Ausdrucks sind Produkte von Operatoren $\tilde{V}(\tau_1)\tilde{V}(\tau_2)$ derart zu ordnen, dass die zeitlich späteren zuerst kommen ($\tau_1 > \tau_2$).

Ein wichtiges Ergebnis ist der Ausdruck (A.15) für den Zeitentwicklungsoperator in erster Ordnung: er ist dann ein einfaches Integral über die Wechselwirkung.

Fermi's Goldene Regel

Wir kehren jetzt zu der ursprünglichen Fragestellung (Gl. A.2) zurück. Die gesuchte Übergangswahrscheinlichkeit enthält das Matrixelement

$$A_{ab} = \langle b|U(t,t_0)|a\rangle = \langle b|U_0(t,t_0)U_I(t,t_0)|a\rangle \tag{A.18}$$

In erster Ordnung wird daraus (die Wirkung von U_0 auf die Zustände $|a,b\rangle$ ist ein Phasenfaktor!)

$$\begin{aligned} A_{ab}^{(1)} &= \frac{e^{-iE_b(t-t_0)/\hbar}}{i\hbar}\int_{t_0}^{t} d\tau\, e^{iE_b(\tau-t_0)/\hbar}\langle b|V(\tau)|a\rangle e^{-iE_a(\tau-t_0)/\hbar} \\ &= \frac{e^{-iE_b(t-t_0)/\hbar}}{i\hbar}\int_{t_0}^{t} d\tau\, e^{i\omega_{ba}(\tau-t_0)}\langle b|V(\tau)|a\rangle \qquad \text{(A.19)} \\ \hbar\omega_{ba} &= E_b - E_a \quad \text{BOHR'SCHE ÜBERGANGSFREQUENZ} \qquad \text{(A.20)} \end{aligned}$$

Hier sehen wir, dass die Übergangswahrscheinlichkeit von einer Art Fouriertransformation des Wechselwirkungsoperators abhängt, wobei genau die Bohr'sche Übergangsfrequenz ins Spiel kommt.

Wir betrachten jetzt eine monochromatische Störung:

$$\hat{V}(t) = Ve^{-i\omega t} + V^{\dagger}e^{i\omega t} \qquad \text{(A.21)}$$

Im oben angeführten Beispiel ist dies der Fall, wenn das Lichtfeld $\mathbf{E}(t)$ eine wohlbestimmte Frequenz hat (z.B. Laserlicht). Dann kann man das Zeitintegral leicht auswerten und findet

$$\begin{aligned} A_{ab}^{(1)} &= \frac{1}{i\hbar}\left(e^{i(\omega_{ba}-\omega)T/2}\langle b|V|a\rangle \frac{\sin((\omega_{ba}-\omega)T/2)}{(\omega_{ba}-\omega)/2} + \right. \\ &\qquad \left. + e^{i(\omega_{ba}+\omega)T/2}\langle b|V^{\dagger}|a\rangle \frac{\sin((\omega_{ba}+\omega)T/2)}{(\omega_{ba}+\omega)/2} \right) \qquad \text{(A.22)} \\ T &= t - t_0 \quad \text{DAUER DER WECHSELWIRKUNG} \qquad \text{(A.23)} \end{aligned}$$

Die Funktion $\sin(\Delta\omega T/2)/(\Delta\omega/2)$, die hier auftritt, besitzt für $\Delta\omega = 0$ einen scharfen Peak der Breite $2\pi/T$ (siehe Abbildung). Für große $|\Delta\omega|$

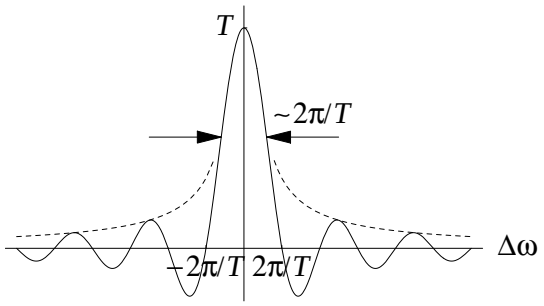

Figure A.1: Die Funktion $\sin(\Delta\omega T/2)/(\Delta\omega/2)$. Gestrichelt die Einhüllende der Oszillationen.

beschreibt sie Oszillationen, deren Amplitude proportional zu $1/|\Delta\omega|$ abfällt.

Als Funktion der Frequenz ω enthält das Matrixelement (A.22) also zwei Peaks an den Stellen $\omega = \pm\omega_{ba}$. Wenn wir annehmen, dass die Dauer der Wechselwirkung genügend groß ist (genauer: $T \gg 2\pi/\omega_{ba}$), sind diese zwei Peaks deutlich voneinander getrennt, und wir erhalten folgenden Ausdruck für die Übergangswahrscheinlichkeit:

$$w_{ab}(t) = \frac{1}{\hbar^2} |\langle b|V|a\rangle|^2 \frac{\sin^2((\omega_{ba}-\omega)T/2)}{(\omega_{ba}-\omega)^2/4} + \frac{1}{\hbar^2} \left|\langle b|V^\dagger|a\rangle\right|^2 \frac{\sin^2((\omega_{ba}+\omega)T/2)}{(\omega_{ba}+\omega)^2/4} \tag{A.24}$$

Die beiden Terme beschreiben zwei verschiedene physikalische Prozesse: im ersten Term wird die Energie E_a des Anfangszustands um ein "Quantum" $\hbar\omega$ vergrößert, so dass

$$E_b = E_a + \hbar\omega \quad \text{ABSORPTION} \tag{A.25}$$

Diese Gleichung läßt sich also im Sinne der Energieerhaltung interpretieren: das System absorbiert ein Energie-Quantum aus dem externen, zeitabhängigen Feld. Umgekehrt beschreibt der zweite Term in (A.24) die Energieerhaltung bei der Emission eines Energie-Quantums:

$$E_b = E_a - \hbar\omega \quad \text{EMISSION} \tag{A.26}$$

Es ist noch zu bemerken, dass für eine endlich große Wechselwirkungszeit T diese Erhaltungssätze nur bis auf Korrekturen der Größenordnung $2\pi\hbar/T$ gelten. Auch dies sollte aus der Fourier-Transformation bekannt sein: Wirkt die Störung nur kurz, ist sie nicht rein monochromatisch und damit das Energie-Quantum nicht scharf bestimmt (Unschärferelation Zeit-Energie).

Resonanzfall. Als erstes Beispiel betrachten wir den Fall, dass die Frequenz der Störung genau auf die Bohrsche Übergangsfrequenz für Absorption abgestimmt ist

$$\hbar\omega = E_b - E_a. \tag{A.27}$$

Die Übergangswahrscheinlichkeit (A.24) wird dann

$$w_{ab}(t) = \frac{1}{\hbar^2} |\langle b|V|a\rangle|^2 T^2 + \frac{1}{\hbar^2} \left|\langle b|V^\dagger|a\rangle\right|^2 \frac{\sin^2(\omega_{ba}T)}{\omega_{ba}^2} \tag{A.28}$$

Der erste Term dominiert bei weitem den zweiten[1], und er wächst quadratisch mit der Zeit T an. Dieses Verhalten ist charakteristisch für

[1] Wir nehmen immer noch eine genügend lange Wechselwirkungszeit $T \gg 2\pi/\omega_{ba}$ an.

den Resonanzfall. Man bezeichnet die Frequenz $\Omega = |\langle b|V|a\rangle|/\hbar$ als RABI-FREQUENZ. Sie gibt die Zeitskala an, auf der die Wahrscheinlichkeit zunimmt, das System im Zustand $|b\rangle$ zu finden. Sie werden später ein Modell kennenlernen, in man sich auf zwei Zustände beschränkt (das "Zwei-Niveau-Atom"). Im Resonanzfall verhalten sich die Wahrscheinlichkeiten $w_a(t)$ und $w_b(t)$ wie $\cos^2(\Omega T)$ und $\sin^2(\Omega T)$. Für eine genügend kleine Rabi-Frequenz findet man den ersten Term der Näherung (A.28) wieder.

Der zweite Term in (A.28) beschreibt einen "nicht-resonanten" Prozess. Weil er die Energieerhaltung verletzt, ist seine Wahrscheinlichkeit sehr klein. Als Funktion von T beschreibt dieser Term Oszillationen mit der Periode $2\pi/\omega_{ba}$. Typischerweise ist es nicht möglich, diese Oszillationen aufzulösen, und deswegen darf man darüber mitteln. Die Wahrscheinlichkeit für den nicht-resonanten Prozess ist damit $\frac{1}{2}|\langle b|V^\dagger|a\rangle|^2/(E_b - E_a)^2$. Weil das Matrixelement der Störung klein gegen die Energien im ungestörten Spektrum ist (Störungstheorie!), ist diese Wahrscheinlichkeit meist vernachlässigbar klein.

Anregung in ein Kontinuum. Als zweites Beispiel kommen wir zu Fermi's Goldener Regel, wie sie in den Büchern angegeben wird. Dazu betrachten wir den Fall, dass das System in ein Kontinuum $|B\rangle$ von Endzuständen in der Nähe des typischen Zustands $|b\rangle$ angeregt wird. Die relevante Größe ist nun die Summe der Übergangswahrscheinlichkeit $w_{ab}(t)$ über die möglichen Endzustände. Diese Summe kann als ein Integral über die Endenergie geschrieben werden

$$w_{a\to B}(t) = \int_{E_f-\varepsilon/2}^{E_f+\varepsilon/2} dE_b\, \rho(E_b) w_{ab}(t). \tag{A.29}$$

Dabei ist $\rho(E_b)$ die ZUSTANDSDICHTE im Energieraum: die Zahl $\rho(E)dE$ ist gleich der Anzahl der Zustände, deren Energie im Intervall $(E, E + dE)$ liegt. In der Wahrscheinlichkeit (A.29) werden alle Endzustände berücksichtigt, deren Energie bei $E_f \equiv E_a + \hbar\omega$ liegt, mit einer Breite ε. Diese Breite gibt die "Energieunschärfe" des Detektors an.

Wir beschränken uns auf den Fall, dass die Energieunschärfe kleiner als die Bohrsche Übergangsfrequenz, aber grösser als die Unschärfe aus der endlichen Wechselwirkungszeit ist:

$$\frac{2\pi\hbar}{T} \ll \varepsilon \ll \omega_{ba} \tag{A.30}$$

Es ist damit ausreichend, im Integral (A.29) nur den resonanten Term in

Gl.(A.24) mitzunehmen, und wir erhalten:

$$w_{a\to B}(t) = \frac{1}{\hbar^2}\int_{E_f-\varepsilon/2}^{E_f+\varepsilon/2} dE_b\,\rho(E_b)\,|\langle b|V|a\rangle|^2\,\frac{\sin^2((\omega_{ba}-\omega)T/2)}{(\omega_{ba}-\omega)^2/4} \qquad \text{(A.31)}$$

Die Funktion mit dem $\sin$ enthält bekanntlich einen scharfen Peak an der Stelle $E_b = E_f = E_a + \hbar\omega$ mit der Breite $2\pi\hbar/T$. Um das Integral auszuwerten, nehmen wir weiter an, dass die Zustandsdichte und das Matrix-Element als Funktion von E_b auf der Skala ε langsam veränderlich sind. Damit können wir sie aus dem Integral herausziehen und erhalten:

$$\begin{aligned} w_{a\to B}(t) &= \frac{1}{\hbar^2}\,|\langle b|V|a\rangle|^2\,\rho(E_f)\int_{E_f-\varepsilon/2}^{E_f+\varepsilon/2} dE_b\,\frac{\sin^2((\omega_{ba}-\omega)T/2)}{(\omega_{ba}-\omega)^2/4} \\ &= \frac{2\pi T}{\hbar}\,|\langle b|V|a\rangle|^2\,\rho(E_f) \qquad \text{(A.32)} \end{aligned}$$

Im letzten Schritt haben wir ausgenutzt, dass der gesamte Peak innerhalb der Energieunschärfe ε liegt und folgendes Integral benutzt:

$$\int_{-\infty}^{+\infty} dx\,\frac{\sin^2 x}{x^2} = \pi \qquad \text{(A.33)}$$

(Beweis: mit Hilfe des Residuensatzes.)

Unser Ergebnis (A.32) zeigt, dass die Übergangswahrscheinlich in ein Kontinuum linear mit T ansteigt. Man beachte den Unterschied zum Resonanzfall. Es bietet sich nun an, eine Übergangsrate einzuführen:

$$\gamma_{a\to B} = \frac{dw_{a\to B}}{dT} = \frac{2\pi}{\hbar}\,|\langle b|V|a\rangle|^2\,\rho(E_f) \qquad \text{(A.34)}$$

Dies ist nun endlich Fermi's Goldene Regel, wie sie in allen Büchern zur Quantenmechanik steht: die Übergangswahrscheinlichkeit in ein Kontinuum ist gleich dem Quadrat des Matrixelements der Störung, multipliziert mit der Zustandsdichte an der Energie des Endzustands.

Beispiel: Born'sche Näherung für den Streuquerschnitt. Eine einfache Anwendung für Fermi's Goldene Regel ist die Streuung eines Teilchens (Elektron, Atom, Lichtwelle) an einem zeitunabhängigen Potential $V(\mathbf{x})$. Die oben ausgeführte Theorie läßt sich auf diesen Fall anwenden, wenn man $\omega = 0$ setzt. In der Tat sind die Anfangs- und Endzustände in der Regel ebene Wellen

$$\langle \mathbf{x}|a\rangle = \frac{e^{i\mathbf{k}_a\cdot\mathbf{x}}}{(2\pi)^{3/2}}, \qquad \text{(A.35)}$$

und diese haben ein kontinuierliches Spektrum. Man betrachtet nun einen Streuprozess, in dem eine Welle mit dem Wellenvektor $\mathbf{k}_a$ auf das Potential auftrifft, gestreut wird und eine gestreute Welle mit dem Wellenvektor $\mathbf{k}_b$ beobachtet wird. Aufgrund der Energieerhaltung gilt $|\mathbf{k}_b| = |\mathbf{k}_a|$ (es sei denn, das Potential $V(\mathbf{x})$ hätte eine unendliche Reichweite).

Die Rate für diesen Prozess ist nun proportional zu

$$|\langle b|V|a\rangle|^2 = \left|\int d^3x\, e^{-i\mathbf{k}_b\cdot\mathbf{x}} V(\mathbf{x}) e^{i\mathbf{k}_a\cdot\mathbf{x}}\right|^2 = \left|\tilde{V}(\Delta\mathbf{k})\right|^2 \tag{A.36}$$

$$\Delta\mathbf{k} = \mathbf{k}_b - \mathbf{k}_a \quad \text{WELLENVEKTORÜBERTRAG} \tag{A.37}$$

Man erhält durch dieses Experiment also die räumlichen Fourierkomponenten des Streupotentials. In einer vollständigen Behandlung berechnet man noch den differentiellen Wirkungsquerschnitt $d\sigma/d\Omega$ (Streuereignisse pro Raumwinkelelement $d\Omega$, pro Zeit und pro einfallendem Fluss). Die Rechnung ist ein wenig kompliziert, weil man die ebenen Wellen geeignet normieren muss, um die Zustandsdichte zu erhalten. Das Ergebnis lautet

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2}|\tilde{V}(\Delta\mathbf{k})|^2. \tag{A.38}$$

Hier ist m die Masse des einfallenden Teilchens.