Feynman Diagrams for Beginners*

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Abstract

We give a short introduction to Feynman diagrams, with many exercises. Text is targeted at students who had little or no prior exposure to quantum field theory. We present condensed description of single-particle Dirac equation, free quantum fields and construction of Feynman amplitude using Feynman diagrams. As an example, we give a detailed calculation of cross-section for annihilation of electron and positron into a muon pair. We also show how such calculations are done with the aid of computer.

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1 Natural units

To describe kinematics of some physical system or event we are free to choose units of measure of the three basic kinematical physical quantities: *length (L)*, *mass (M)* and *time (T)*. Equivalently, we may choose any three linearly independent combinations of these quantities. The choice of L, T and M is usually made (e.g. in SI system of units) because they are most convenient for description of our immediate experience. However, elementary particles experience a different world, one governed by the laws of relativistic quantum mechanics.

Natural units in relativistic quantum mechanics are chosen in such a way that fundamental constants of this theory, c and $\hbar$, are both equal to one. $[c] = LT^{-1}$, $[\hbar] = ML^{-2}T^{-1}$, and to completely fix our system of units we specify the unit of energy (ML^2T^{-2}):

$$1\,\text{GeV} = 1.6 \cdot 10^{-10}\,\text{kg m}^2\,\text{s}^{-2}\ ,$$

approximately equal to the mass of the proton. What we do in practice is:

- we ignore $\hbar$ and c in formulae and only restore them at the end (if at all)
- we measure *everything* in GeV, GeV^{-1}, GeV^2, ...

Example: *Thomson cross section*

Total cross section for scattering of classical electromagnetic radiation by a free electron (Thomson scattering) is, in natural units,

$$\sigma_{\text{T}} = \frac{8\pi\alpha^2}{3m_e^2}\ . \tag{1}$$

To restore $\hbar$ and c we insert them in the above equation with general powers α and β, which we determine by requiring that cross section has the dimension of area

(L^2):

$$\sigma_{\mathrm{T}} = \frac{8\pi\alpha^2}{3m_e^2}\hbar^\alpha c^\beta \tag{2}$$

$$[\sigma] = L^2 = \frac{1}{M^2}(ML^2T^{-1})^\alpha(LT^{-1})^\beta$$

$$\Rightarrow\ \alpha = 2\ , \quad \beta = -2\ ,$$

i.e.

$$\sigma_{\mathrm{T}} = \frac{8\pi\alpha^2}{3m_e^2}\frac{\hbar^2}{c^2} = 0.665\cdot 10^{-24}\,\mathrm{cm}^2 = 665\,\mathrm{mb}\ . \tag{3}$$

Linear independence of $\hbar$ and c implies that this can always be done in a unique way. ■

Following conversion relations are often useful:

$$\begin{aligned}
1\,\mathrm{fermi} &= 5.07\,\mathrm{GeV}^{-1}\\
1\,\mathrm{GeV}^{-2} &= 0.389\,\mathrm{mb}\\
1\,\mathrm{GeV}^{-1} &= 6.582\cdot 10^{-25}\,\mathrm{s}\\
1\,\mathrm{kg} &= 5.61\cdot 10^{26}\,\mathrm{GeV}\\
1\,\mathrm{m} &= 5.07\cdot 10^{15}\,\mathrm{GeV}^{-1}\\
1\,\mathrm{s} &= 1.52\cdot 10^{24}\,\mathrm{GeV}^{-1}
\end{aligned}$$

Exercise 1 Check these relations.

Calculating with GeVs is much more elegant. Using m_e = 0.511·10^{-3} GeV we get

$$\sigma_{\mathrm{T}} = \frac{8\pi\alpha^2}{3m_e^2} = 1709\,\mathrm{GeV}^{-2} = 665\,\mathrm{mb}\ . \tag{4}$$

right away.

Exercise 2 The decay width of the π^0 particle is

$$\Gamma = \frac{1}{\tau} = 7.7\,\mathrm{eV}. \tag{5}$$

Calculate its lifetime τ in seconds. (By the way, particle's half-life is equal to $\tau\ln 2$.)

2 Single-particle Dirac equation

2.1 The Dirac equation

Turning the relativistic energy equation

$$E^2 = \boldsymbol{p}^2 + m^2 \ . \tag{6}$$

into a differential equation using the usual substitutions

$$\boldsymbol{p} \to -i\nabla \ , \quad E \to i\frac{\partial}{\partial t} \ , \tag{7}$$

results in the Klein-Gordon equation:

$$(\Box + m^2)\psi(x) = 0 \ , \tag{8}$$

which, interpreted as a single-particle wave equation, has problematic negative energy solutions. This is due to the negative root in $E = \pm\sqrt{\boldsymbol{p}^2 + m^2}$. Namely, in relativistic *mechanics* this negative root could be ignored, but in quantum physics one must keep *all* of the complete set of solutions to a differential equation.

In order to overcome this problem Dirac tried the ansatz*

$$(i\beta^\mu\partial_\mu + m)(i\gamma^\nu\partial_\nu - m)\psi(x) = 0 \tag{9}$$

with β^μ and γ^ν to be determined by requiring consistency with the Klein-Gordon equation. This requires $\gamma^\mu = \beta^\mu$ and

$$\gamma^\mu\partial_\mu\gamma^\nu\partial_\nu = \partial^\mu\partial_\mu \ , \tag{10}$$

which in turn implies

$$(\gamma^0)^2 = 1 \ , \quad (\gamma^i)^2 = -1 \ ,$$
$$\{\gamma^\mu, \gamma^\nu\} \equiv \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 0 \quad \text{for } \mu \neq \nu \ .$$

This can be compactly written in form of the *anticommutation relations*

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \ , \quad g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \ . \tag{11}$$

These conditions are obviously impossible to satisfy with γ's being equal to usual numbers, but we can satisfy them by taking γ's equal to (at least) four-by-four matrices.

* *ansatz*: guess, trial solution (from German *Ansatz*: start, beginning, onset, attack)

Now, to satisfy (9) it is enough that one of the two factors in that equation is zero, and by convention we require this from the second one. Thus we obtain the *Dirac equation*:

$$(i\gamma^\mu\partial_\mu - m)\psi(x) = 0 \ . \tag{12}$$

$\psi(x)$ now has four components and is called the *Dirac spinor*.

One of the most frequently used representations for γ matrices is the original Dirac representation

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \ , \tag{13}$$

where σ^i are the Pauli matrices:

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ . \tag{14}$$

This representation is very convenient for the non-relativistic approximation, since then the dominant energy terms $(i\gamma^0\partial_0 - \ldots - m)\psi(0)$ turn out to be diagonal.

Two other often used representations are

- the Weyl (or chiral) representation — convenient in the ultra-relativistic regime (where $E \gg m$)
- the Majorana representation — makes the Dirac equation real; convenient for *Majorana fermions* for which antiparticles are equal to particles

(*Question:* Why can we choose at most one γ matrix to be diagonal?)

Properties of the Pauli matrices:

$$\sigma^{i\dagger} = \sigma^i \tag{15}$$
$$\sigma^{i*} = (i\sigma^2)\sigma^i(i\sigma^2) \tag{16}$$
$$[\sigma^i, \sigma^j] = 2i\epsilon^{ijk}\sigma^k \tag{17}$$
$$\{\sigma^i, \sigma^j\} = 2\delta^{ij} \tag{18}$$
$$\sigma^i\sigma^j = \delta^{ij} + i\epsilon^{ijk}\sigma^k \tag{19}$$

where ϵ^{ijk} is the totally antisymmetric Levi-Civita tensor ($\epsilon^{123} = \epsilon^{231} = \epsilon^{312} = 1$, $\epsilon^{213} = \epsilon^{321} = \epsilon^{132} = -1$, and all other components are zero).

Exercise 3 Prove that $(\boldsymbol{\sigma} \cdot \boldsymbol{a})^2 = \boldsymbol{a}^2$ for any three-vector $\boldsymbol{a}$.

Exercise 4 Using properties of the Pauli matrices, prove that γ matrices in the Dirac representation satisfy $\{\gamma^i, \gamma^j\} = 2g^{ij} = -2\delta^{ij}$, in accordance with the anticommutation relations. (Other components of the anticommutation relations, $(\gamma^0)^2 = 1$, $\{\gamma^0, \gamma^i\} = 0$, are trivial to prove.)

Exercise 5 Show that in the Dirac representation $\gamma^0\gamma^\mu\gamma^0 = \gamma^{\mu\dagger}$.

Exercise 6 Determine the Dirac Hamiltonian by writing the Dirac equation in the form $i\partial\psi/\partial t = H\psi$. Show that the hermiticity of the Dirac Hamiltonian implies that the relation from the previous exercise is valid regardless of the representation.

The *Feynman slash* notation, $\not{a} \equiv a_\mu\gamma^\mu$, is often used.

2.2 The adjoint Dirac equation and the Dirac current

For constructing the Dirac current we need the equation for $\psi(x)^\dagger$. By taking the Hermitian adjoint of the Dirac equation we get

$$\psi^\dagger\gamma^0(i\overleftarrow{\not{\partial}} + m) = 0 \ ,$$

and we define the *adjoint* spinor $\bar{\psi} \equiv \psi^\dagger\gamma^0$ to get the *adjoint Dirac equation*

$$\bar{\psi}(x)(i\overleftarrow{\not{\partial}} + m) = 0 \ .$$

$\bar{\psi}$ is introduced not only to get aesthetically pleasing equations but also because it can be shown that, unlike $\psi^\dagger$, it transforms covariantly under the Lorentz transformations.

Exercise 7 Check that the current $j^\mu = \bar{\psi}\gamma^\mu\psi$ is conserved, i.e. that it satisfies the continuity relation $\partial_\mu j^\mu = 0$.

Components of this relativistic four-current are $j^\mu = (\rho, \boldsymbol{j})$. Note that $\rho = j^0 = \bar{\psi}\gamma^0\psi = \psi^\dagger\psi > 0$, i.e. that probability is positive definite, as it must be.

2.3 Free-particle solutions of the Dirac equation

Since we are preparing ourselves for the perturbation theory calculations, we need to consider only free-particle solutions. For solutions in various potentials, see the literature.

The fact that Dirac spinors satisfy the Klein-Gordon equation suggests the ansatz

$$\psi(x) = u(\boldsymbol{p})e^{-ipx} \ , \tag{20}$$

which after inclusion in the Dirac equation gives the *momentum space Dirac equation*

$$(\not{p} - m)u(\boldsymbol{p}) = 0 \ . \tag{21}$$

This has two positive-energy solutions

$$u(\boldsymbol{p}, \sigma) = N \begin{pmatrix} \chi^{(\sigma)} \\ \dfrac{\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E+m} \chi^{(\sigma)} \end{pmatrix} \ , \quad \sigma = 1, 2 \ , \tag{22}$$

where

$$\chi^{(1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ , \quad \chi^{(2)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ , \tag{23}$$

and two negative-energy solutions which are then interpreted as positive-energy *antiparticle* solutions

$$v(\boldsymbol{p}, \sigma) = -N \begin{pmatrix} \dfrac{\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E+m} (i\sigma^2)\chi^{(\sigma)} \\ (i\sigma^2)\chi^{(\sigma)} \end{pmatrix} \ , \quad \sigma = 1, 2, \qquad E > 0 \ . \tag{24}$$

N is the normalization constant to be determined later. Spinors above agree with those of [1]. The momentum-space Dirac equation for antiparticle solutions is

$$(\not{p} + m)v(\boldsymbol{p}, \sigma) = 0 \ . \tag{25}$$

It can be shown that the two solutions, one with $\sigma = 1$ and another with $\sigma = 2$, correspond to the two spin states of the spin-1/2 particle.

Exercise 8 Determine momentum-space Dirac equations for $\bar{u}(\boldsymbol{p}, \sigma)$ and $\bar{v}(\boldsymbol{p}, \sigma)$.

Normalization

In non-relativistic single-particle quantum mechanics normalization of a wave-function is straightforward. Probability that the particle is somewhere in space is equal to one, and this translates into the normalization condition $\int \psi^* \psi \, dV = 1$. On the other hand, we will eventually use spinors (22) and (24) in many-particle quantum field theory so their normalization is not unique. We will choose normalization convention where we have $2E$ particles in the unit volume:

$$\int\limits_{\text{unit volume}} \rho \, dV = \int\limits_{\text{unit volume}} \psi^\dagger \psi \, dV = 2E \tag{26}$$

This choice is relativistically covariant because the Lorentz contraction of the volume element is compensated by the energy change. There are other normalization conventions with other advantages.

Exercise 9 Determine the normalization constant N conforming to this choice.

Completeness

Exercise 10 Using the explicit expressions (22) and (24) show that

$$\sum_{\sigma=1,2} u(\boldsymbol{p},\sigma)\bar{u}(\boldsymbol{p},\sigma) = \not{p} + m \ , \tag{27}$$

$$\sum_{\sigma=1,2} v(\boldsymbol{p},\sigma)\bar{v}(\boldsymbol{p},\sigma) = \not{p} - m \ . \tag{28}$$

These relations are often needed in calculations of Feynman diagrams with unpolarized fermions. See later sections.

Parity and bilinear covariants

The parity transformation:

- $P : \boldsymbol{x} \to -\boldsymbol{x}, t \to t$
- $P : \psi \to \gamma^0\psi$

Exercise 11 Check that the current $j^\mu = \bar{\psi}\gamma^\mu\psi$ transforms as a vector under parity i.e. that $j^0 \to j^0$ and $\boldsymbol{j} \to -\boldsymbol{j}$.

Any fermion current will be of the form $\bar{\psi}\Gamma\psi$, where Γ is some four-by-four matrix. For construction of interaction Lagrangian we want to use only those currents that have definite Lorentz transformation properties. To this end we first define two new matrices:

$$\gamma^5 \equiv i\gamma^0\gamma^1\gamma^2\gamma^3 \overset{\text{Dirac rep.}}{=} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \quad \{\gamma^5, \gamma^\mu\} = 0 \ , \tag{29}$$

$$\sigma^{\mu\nu} \equiv \frac{i}{2}[\gamma^\mu, \gamma^\nu] \ , \quad \sigma^{\mu\nu} = -\sigma^{\nu\mu} \ . \tag{30}$$

Now $\bar{\psi}\Gamma\psi$ will transform covariantly if Γ is one of the matrices given in the following table. Transformation properties of $\bar{\psi}\Gamma\psi$, the number of different γ

matrices in Γ, and the number of components of Γ are also displayed.

Γ	transforms as	# of γ's	# of components
1	scalar	0	1
γ^μ	vector	1	4
$\sigma^{\mu\nu}$	tensor	2	6
$\gamma^5\gamma^\mu$	axial vector	3	4
γ^5	pseudoscalar	4	1

This exhausts all possibilities. The total number of components is 16, meaning that the set $\{1, \gamma^\mu, \sigma^{\mu\nu}, \gamma^5\gamma^\mu, \gamma^5\}$ makes a complete basis for any four-by-four matrix. Such $\bar{\psi}\Gamma\psi$ currents are called *bilinear covariants*.

3 Free quantum fields

Single-particle Dirac equation is (a) not exactly right even for single-particle systems such as the H-atom, and (b) unable to treat many-particle processes such as the β-decay $n \to p\, e^- \bar{\nu}$. We have to upgrade to quantum field theory.

Any Dirac field is some superposition of the complete set

$$u(\boldsymbol{p}, \sigma)e^{-ipx} \ , \quad v(\boldsymbol{p}, \sigma)e^{ipx} \ , \quad \sigma = 1, 2, \quad \boldsymbol{p} \in \mathbb{R}^3$$

and we can write it as

$$\psi(x) = \sum_\sigma \int \frac{d^3p}{\sqrt{(2\pi)^3 2E}} \left[u(\boldsymbol{p}, \sigma)a(\boldsymbol{p}, \sigma)e^{-ipx} + v(\boldsymbol{p}, \sigma)a^{c\dagger}(\boldsymbol{p}, \sigma)e^{ipx} \right] \ . \quad (31)$$

Here $1/\sqrt{(2\pi)^3 2E}$ is a normalization factor (there are many different conventions), and $a(\boldsymbol{p}, \sigma)$ and $a^{c\dagger}(\boldsymbol{p}, \sigma)$ are expansion coefficients. To make this a *quantum Dirac field* we promote these coefficients to the rank of operators by imposing the *anticommutation* relations

$$\{a(\boldsymbol{p}, \sigma), a^\dagger(\boldsymbol{p}', \sigma')\} = \delta_{\sigma\sigma'}\delta^3(\boldsymbol{p} - \boldsymbol{p}'), \quad (32)$$

and similarly for $a^c(\boldsymbol{p}, \sigma)$. (For bosonic fields we would have a *commutation* relations instead.) This is similar to the promotion of position and momentum to the rank of operators by the $[x_i, p_j] = i\hbar\delta_{ij}$ commutation relations, which is why is this transition from the single-particle quantum theory to the quantum field theory sometimes called *second quantization*.

Operator $a^\dagger$, when operating on vacuum state $|0\rangle$, creates one-particle state $|\boldsymbol{p}, \sigma\rangle$

$$a^\dagger(\boldsymbol{p}, \sigma)|0\rangle = |\boldsymbol{p}, \sigma\rangle \ , \quad (33)$$

and this is the reason that it is named a *creation* operator. Similarly, a is an *annihilation* operator

$$a(\boldsymbol{p},\sigma)|\boldsymbol{p},\sigma\rangle = |0\rangle \ , \tag{34}$$

and $a^{c\dagger}$ and a^c are creation and annihilation operators for antiparticle states (c in a^c stands for "conjugated").

Processes in particle physics are mostly calculated in the framework of the theory of such fields — *quantum field theory*. This theory can be described at various levels of rigor but in any case is complicated enough to be beyond the scope of these notes.

However, predictions of quantum field theory pertaining to the elementary particle interactions can often be calculated using a relatively simple "recipe" — *Feynman diagrams*.

Before we turn to describing the method of Feynman diagrams, let us just specify other quantum fields that take part in the elementary particle physics interactions. All these are *free* fields, and interactions are treated as their perturbations. Each particle type (electron, photon, Higgs boson, ...) has its own quantum field.

3.1 Spin 0: scalar field

E.g. Higgs boson, pions, ...

$$\phi(x) = \int \frac{d^3p}{\sqrt{(2\pi)^3 2E}} \left[a(\boldsymbol{p})e^{-ipx} + a^{c\dagger}(\boldsymbol{p})e^{ipx}\right] \tag{35}$$

3.2 Spin 1/2: the Dirac field

E.g. quarks, leptons

We have already specified the Dirac spin-1/2 field. There are other types: Weyl and Majorana spin-1/2 fields but they are beyond our scope.

3.3 Spin 1: vector field

Either

- massive (e.g. W,Z weak bosons) or
- massless (e.g. photon)

$$A^\mu(x) = \sum_\lambda \int \frac{d^3p}{\sqrt{(2\pi)^3 2E}} \left[\epsilon^\mu(\boldsymbol{p},\lambda)a(\boldsymbol{p},\lambda)e^{-ipx} + \epsilon^{\mu *}(\boldsymbol{p},\lambda)a^\dagger(\boldsymbol{p},\lambda)e^{ipx}\right] \tag{36}$$

$\epsilon^\mu(\boldsymbol{p},\lambda)$ is a polarization vector. For massive particles it obeys

$$p_\mu \epsilon^\mu(\boldsymbol{p},\lambda) = 0 \tag{37}$$

automatically, whereas in the massless case this condition can be imposed thanks to gauge invariance (Lorentz gauge condition). This means that there are only three independent polarizations of a massive vector particle: $\lambda = 1,2,3$ or $\lambda = +,-,0$. In massless case gauge symmetry can be further exploited to eliminate one more polarization state leaving us with only two: $\lambda = 1,2$ or $\lambda = +,-$.

Normalization of polarization vectors is such that

$$\epsilon^*(\boldsymbol{p},\lambda)\cdot\epsilon(\boldsymbol{p},\lambda) = -1\ . \tag{38}$$

E.g. for a massive particle moving along the z-axis ($p = (E,0,0,|\boldsymbol{p}|)$) we can take

$$\epsilon(\boldsymbol{p},\pm) = \mp\frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ \pm i \\ 0 \end{pmatrix}\ , \quad \epsilon(\boldsymbol{p},0) = \frac{1}{m}\begin{pmatrix} |\boldsymbol{p}| \\ 0 \\ 0 \\ E \end{pmatrix} \tag{39}$$

Exercise 12 Calculate

$$\sum_\lambda \epsilon^{\mu *}(\boldsymbol{p},\lambda)\epsilon^\nu(\boldsymbol{p},\lambda)$$

Hint: Write it in the most general form $(Ag^{\mu\nu} + Bp^\mu p^\nu)$ and then determine A and B.

The obtained result obviously cannot be simply extrapolated to the massless case via the limit $m \to 0$. Gauge symmetry makes massless polarization sum somewhat more complicated but for the purpose of the simple Feynman diagram calculations it is permissible to use just the following relation

$$\sum_\lambda \epsilon^{\mu *}(\boldsymbol{p},\lambda)\epsilon^\nu(\boldsymbol{p},\lambda) = -g^{\mu\nu}\ .$$

4 Golden rules for decays and scatterings

Principal experimental observables of particle physics are

- scattering cross section $\sigma(1+2 \to 1' + 2' + \cdots + n')$
- decay width $\Gamma(1 \to 1' + 2' + \cdots + n')$

On the other hand, theory is defined in terms of Lagrangian density of quantum fields, e.g.

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \frac{g}{4!}\phi^4 \ .$$

How to calculate σ's and Γ's from $\mathcal{L}$?

To calculate rate of transition from the state $|\alpha\rangle$ to the state $|\beta\rangle$ in the presence of the interaction potential V_I in non-relativistic quantum theory we have the Fermi's Golden Rule

$$\begin{pmatrix} \alpha \to \beta \\ \text{transition rate} \end{pmatrix} = \frac{2\pi}{\hbar}|\langle\beta|V_I|\alpha\rangle|^2 \times \begin{pmatrix} \text{density of final} \\ \text{quantum states} \end{pmatrix} . \tag{40}$$

This is in the lowest order perturbation theory. For higher orders we have terms with products of more interaction potential matrix elements $\langle|V_I|\rangle$.

In quantum field theory there is a counterpart to these matrix elements — the *S-matrix*:

$$\langle\beta|V_I|\alpha\rangle + \big(\text{higher-order terms}\big) \quad \longrightarrow \quad \langle\beta|S|\alpha\rangle \ . \tag{41}$$

On one side, S-matrix elements can be perturbatively calculated (knowing the interaction Lagrangian/Hamiltonian) with the help of the *Dyson series*

$$S = 1 - i\int d^4x_1\,\mathcal{H}(x_1) + \frac{(-i)^2}{2!}\int d^4x_1\,d^4x_2\,T\{\mathcal{H}(x_1)\mathcal{H}(x_2)\} + \cdots \ , \tag{42}$$

and on another, we have "golden rules" that associate these matrix elements with cross-sections and decay widths.

It is convenient to express these golden rules in terms of the *Feynman invariant amplitude* $\mathcal{M}$ which is obtained by stripping some kinematical factors off the S-matrix:

$$\langle\beta|S|\alpha\rangle = \delta_{\beta\alpha} - i(2\pi)^4\delta^4(p_\beta - p_\alpha)\mathcal{M}_{\beta\alpha}\prod_{i=\alpha,\beta}\frac{1}{\sqrt{(2\pi)^3\,2E_i}} \ . \tag{43}$$

Now we have two rules:

- Partial decay rate of $1 \to 1' + 2' + \cdots + n'$

$$d\Gamma = \frac{1}{2E_1}\overline{|\mathcal{M}_{\beta\alpha}|^2}\,(2\pi)^4\delta^4(p_1 - p_1' - \cdots - p_n')\prod_{i=1}^{n}\frac{d^3p_i'}{(2\pi)^3\,2E_i'} \ , \tag{44}$$

- Differential cross section for a scattering $1 + 2 \to 1' + 2' + \cdots + n'$

$$d\sigma = \frac{1}{u_\alpha}\frac{1}{2E_1}\frac{1}{2E_2}\overline{|\mathcal{M}_{\beta\alpha}|^2}\,(2\pi)^4\delta^4(p_1 + p_2 - p_1' - \cdots - p_n')\prod_{i=1}^{n}\frac{d^3p_i'}{(2\pi)^3\,2E_i'} \ , \tag{45}$$

where u_α is the relative velocity of particles 1 and 2:

$$u_\alpha = \frac{\sqrt{(p_1 \cdot p_2)^2 - m_1^2 m_2^2}}{E_1 E_2} \,, \tag{46}$$

and $\overline{|\mathcal{M}|^2}$ is the Feynman invariant amplitude averaged over unmeasured particle spins (see Section 6.1). The dimension of $\mathcal{M}$, in units of energy, is

- for decays $[\mathcal{M}] = 3 - n$
- for scattering of two particles $[\mathcal{M}] = 2 - n$

where n is the number of produced particles.

So calculation of some observable quantity consists of two stages:

1. Determination of $\overline{|\mathcal{M}|^2}$. For this we use the method of Feynman diagrams to be introduced in the next section.
2. Integration over the Lorentz invariant phase space

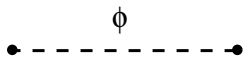
$$d\text{Lips} = (2\pi)^4 \delta^4(p_1 + p_2 - p_1' - \cdots - p_n') \prod_{i=1}^{n} \frac{d^3 p_i'}{(2\pi)^3 \, 2E_i'} \,.$$

5 Feynman diagrams

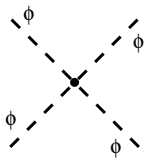
Example: ϕ^4-*theory*

$$\mathcal{L} = \frac{1}{2}\partial_\mu \phi \partial^\mu \phi - \frac{1}{2} m^2 \phi^2 - \frac{g}{4!}\phi^4$$

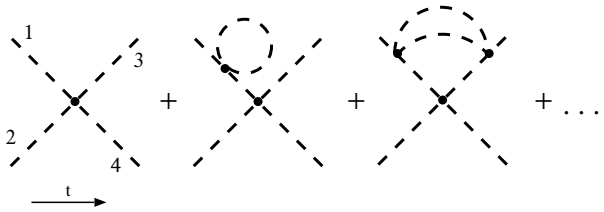
- Free (kinetic) Lagrangian (terms with exactly two fields) determines particles of the theory and their propagators. Here we have just one scalar field:



- Interaction Lagrangian (terms with three or more fields) determines possible vertices. Here, again, there is just one vertex:



We construct all possible diagrams with fixed outer particles. E.g. for scattering of two scalar particles in this theory we would have

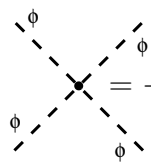
$\mathcal{M}(1+2\to 3+4) =$ 

In these diagrams time flows from left to right. Some people draw Feynman diagrams with time flowing up, which is more in accordance with the way we usually draw space-time in relativity physics.

Since each vertex corresponds to one interaction Lagrangian (Hamiltonian) term in (42), diagrams with loops correspond to higher orders of perturbation theory. Here we will work only to the lowest order, so we will use *tree diagrams* only.

To actually write down the Feynman amplitude $\mathcal{M}$, we have a set of *Feynman rules* that associate factors with elements of the Feynman diagram. In particular, to get $-i\mathcal{M}$ we construct the Feynman rules in the following way:

- the vertex factor is just the i times the interaction term in the (momentum space) Lagrangian with all fields removed:

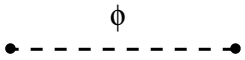
$$i\mathcal{L}_{\mathrm{I}} = -i\frac{g}{4!}\phi^4 \quad \overset{\text{removing fields}}{\Rightarrow} \quad$$ 

$$= -i\frac{g}{4!} \tag{47}$$

- the propagator is i times the inverse of the kinetic operator (defined by the free equation of motion) in the momentum space:

$$\mathcal{L}_{\text{free}} \overset{\text{Euler-Lagrange eq.}}{\longrightarrow} (\partial_\mu\partial^\mu + m^2)\phi = 0 \qquad \text{(Klein-Gordon eq.)} \tag{48}$$

Going to the momentum space using the substitution $\partial^\mu \to -ip^\mu$ and then taking the inverse gives:

$$(p^2 - m^2)\phi = 0 \quad \Rightarrow \quad$$ 

$$= \frac{i}{p^2 - m^2} \tag{49}$$

(Actually, the correct Feynman propagator is $i/(p^2 - m^2 + i\epsilon)$, but for our purposes we can ignore the infinitesimal $i\epsilon$ term.)

- External lines are represented by the appropriate polarization vector or spinor (the one that stands by the appropriate creation or annihilation operator in the fields (31), (35), (36) and their conjugates):

particle	Feynman rule
ingoing fermion	u
outgoing fermion	$\bar{u}$
ingoing antifermion	$\bar{v}$
outgoing antifermion	v
ingoing photon	ϵ^{μ}
outgoing photon	$\epsilon^{\mu *}$
ingoing scalar	1
outgoing scalar	1

So the tree-level contribution to the scalar-scalar scattering amplitude in this ϕ^4 theory would be just

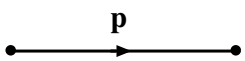
$$-i\mathcal{M} = -i\frac{g}{4!} \ . \tag{50}$$

■

Exercise 13 Determine the Feynman rules for the electron propagator and for the only vertex of quantum electrodynamics (QED):

$$\mathcal{L} = \bar{\psi}(i\partial\!\!\!/ + eA\!\!\!/ - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \qquad F^{\mu\nu} = \partial^{\mu}A^{\nu} - \partial^{\nu}A^{\mu} \ . \tag{51}$$

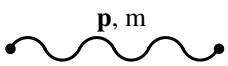
Note that also



$$= \frac{i\sum_{\sigma} u(\boldsymbol{p},\sigma)\bar{u}(\boldsymbol{p},\sigma)}{p^2 - m^2} \ , \tag{52}$$

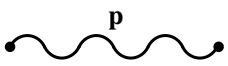
i.e. the electron propagator is just the scalar propagator multiplied by the polarization sum. It is nice that this generalizes to propagators of all particles. This is very helpful since inverting the photon kinetic operator is non-trivial due to gauge symmetry complications. Hence, propagators of vector particles are

massive:



$$= \frac{-i\left(g^{\mu\nu} - \dfrac{p^{\mu}p^{\nu}}{m^2}\right)}{p^2 - m^2} \ , \tag{53}$$

massless:



$$= \frac{-ig^{\mu\nu}}{p^2} \ . \tag{54}$$

This is in principle *almost* all we need to know to be able to calculate the Feynman amplitude of any given process. Note that propagators and external-line polarization vectors are determined only by the particle type (its spin and mass) so that the corresponding rules above are not restricted only to the ϕ^4 theory and QED, but will apply to all theories of scalars, spin-1 vector bosons and Dirac fermions (such as the standard model). The only additional information we need are the vertex factors.

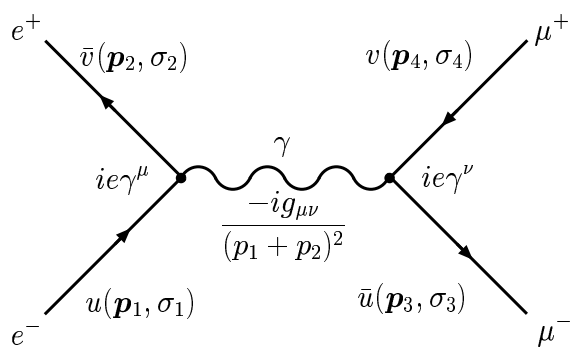
"Almost" in the preceding paragraph alludes to the fact that in general Feynman diagram calculation there are several additional subtleties:

- In loop diagrams some internal momenta are undetermined and we have to integrate over those. Also, there is an additional factor (-1) for each closed fermion loop. Since we will consider tree-level diagrams only, we can ignore this.
- There are some combinatoric numerical factors when identical fields come into a single vertex.
- Sometimes there is a relative (-) sign between diagrams.
- There is a symmetry factor if there are identical particles in the final state.

For explanation of these, reader is advised to look in some quantum field theory textbook.

6 Example: $e^+e^- \to \mu^+\mu^-$ in QED

There is only one contributing tree-level diagram:



We write down the amplitude using the Feynman rules of QED and following

fermion lines backwards. Order of lines themselves is unimportant.

$$-i\mathcal{M} = [\bar{u}(\boldsymbol{p}_3,\sigma_3)(ie\gamma^\nu)v(\boldsymbol{p}_4,\sigma_4)]\,\frac{-ig_{\mu\nu}}{(p_1+p_2)^2}\,[\bar{v}(\boldsymbol{p}_2,\sigma_2)(ie\gamma^\mu)u(\boldsymbol{p}_1,\sigma_1)]\ , \tag{55}$$

or, introducing abbreviation $u_1 \equiv u(\boldsymbol{p}_1,\sigma_1)$,

$$\mathcal{M} = \frac{e^2}{(p_1+p_2)^2}[\bar{u}_3\gamma_\mu v_4][\bar{v}_2\gamma^\mu u_1]\ . \tag{56}$$

Exercise 14 Draw Feynman diagram(s) and write down the amplitude for Compton scattering $\gamma e^- \to \gamma e^-$.

6.1 Summing over polarizations

If we knew momenta and polarizations of all external particles, we could calculate $\mathcal{M}$ explicitly. However, experiments are often done with unpolarized particles so we have to sum over the polarizations (spins) of the final particles and average over the polarizations (spins) of the initial ones:

$$|\mathcal{M}|^2 \to \overline{|\mathcal{M}|^2} = \underbrace{\frac{1}{2}\,\frac{1}{2}\sum_{\sigma_1\sigma_2}}_{\text{avg. over initial pol.}}\ \overbrace{\sum_{\sigma_3\sigma_4}}^{\text{sum over final pol.}}\ |\mathcal{M}|^2\ . \tag{57}$$

Factors $1/2$ are due to the fact that each initial fermion has two polarization (spin) states.
(*Question:* Why we sum probabilities and not amplitudes?)

In the calculation of $|\mathcal{M}|^2 = \mathcal{M}^*\mathcal{M}$, the following identity is needed

$$[\bar{u}\gamma^\mu v]^* = [u^\dagger\gamma^0\gamma^\mu v]^\dagger = v^\dagger\gamma^{\mu\dagger}\gamma^0 u = [\bar{v}\gamma^\mu u]\ . \tag{58}$$

Thus,

$$\overline{|\mathcal{M}|^2} = \frac{e^4}{4(p_1+p_2)^4}\sum_{\sigma_{1,2,3,4}}[\bar{v}_4\gamma_\mu u_3][\bar{u}_1\gamma^\mu v_2][\bar{u}_3\gamma_\nu v_4][\bar{v}_2\gamma^\nu u_1]\ . \tag{59}$$

6.2 Casimir trick

Sums over polarizations are easily performed using the following trick. First we write $\sum[\bar{u}_1\gamma^\mu v_2][\bar{v}_2\gamma^\nu u_1]$ with explicit spinor indices $\alpha, \beta, \gamma, \delta = 1, 2, 3, 4$:

$$\sum_{\sigma_1\sigma_2} \bar{u}_{1\alpha}\gamma^\mu_{\alpha\beta} v_{2\beta}\ \bar{v}_{2\gamma}\gamma^\nu_{\gamma\delta} u_{1\delta}\ . \tag{60}$$

We can now move $u_{1\delta}$ to the front ($u_{1\delta}$ is just a number, element of u_1 vector, so it commutes with everything), and then use the completeness relations (27) and (28),

$$\begin{aligned} \sum_{\sigma_1} u_{1\delta}\,\bar{u}_{1\alpha} &= (\not{p}_1 + m_1)_{\delta\alpha}\ , \\ \sum_{\sigma_2} v_{2\beta}\,\bar{v}_{2\gamma} &= (\not{p}_2 - m_2)_{\beta\gamma}\ , \end{aligned}$$

which turn sum (60) into

$$(\not{p}_1 + m_1)_{\delta\alpha}\,\gamma^\mu_{\alpha\beta}\,(\not{p}_2 - m_2)_{\beta\gamma}\,\gamma^\nu_{\gamma\delta} = \mathrm{Tr}[(\not{p}_1 + m_1)\gamma^\mu(\not{p}_2 - m_2)\gamma^\nu]\ . \tag{61}$$

This means that

$$\overline{|\mathcal{M}|^2} = \frac{e^4}{4(p_1+p_2)^4}\mathrm{Tr}[(\not{p}_1 + m_1)\gamma^\mu(\not{p}_2 - m_2)\gamma^\nu]\,\mathrm{Tr}[(\not{p}_4 - m_4)\gamma_\mu(\not{p}_3 + m_3)\gamma_\nu]\ . \tag{62}$$

Thus we got rid off all the spinors and we are left only with traces of γ matrices. These can be evaluated using the relations from the following section.

6.3 Traces and contraction identities of γ matrices

All are consequence of the anticommutation relations $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$, $\{\gamma^\mu, \gamma^5\} = 0$, $(\gamma^5)^2 = 1$, and of nothing else!

Trace identities

1. Trace of an odd number of γ's vanishes:

$$\begin{aligned} \mathrm{Tr}(\gamma^{\mu_1}\gamma^{\mu_2}\cdots\gamma^{\mu_{2n+1}}) &= \mathrm{Tr}(\gamma^{\mu_1}\gamma^{\mu_2}\cdots\gamma^{\mu_{2n+1}}\overbrace{\gamma^5\gamma^5}^{1}) \\ \text{(moving } \gamma^5 \text{ over each } \gamma^{\mu_i}) &= -\mathrm{Tr}(\gamma^5\gamma^{\mu_1}\gamma^{\mu_2}\cdots\gamma^{\mu_{2n+1}}\gamma^5) \\ \text{(cyclic property of trace)} &= -\mathrm{Tr}(\gamma^{\mu_1}\gamma^{\mu_2}\cdots\gamma^{\mu_{2n+1}}\gamma^5\gamma^5) \\ &= -\mathrm{Tr}(\gamma^{\mu_1}\gamma^{\mu_2}\cdots\gamma^{\mu_{2n+1}}) \\ &= 0 \end{aligned}$$

2. Tr 1 = 4

3. $$\mathrm{Tr}\gamma^\mu\gamma^\nu = \mathrm{Tr}(2g^{\mu\nu} - \gamma^\nu\gamma^\mu) \overset{(2.)}{=} 8g^{\mu\nu} - \mathrm{Tr}\gamma^\nu\gamma^\mu = 8g^{\mu\nu} - \mathrm{Tr}\gamma^\mu\gamma^\nu$$
$$\Rightarrow\ 2\mathrm{Tr}\gamma^\mu\gamma^\nu = 8g^{\mu\nu}\ \Rightarrow\ \mathrm{Tr}\gamma^\mu\gamma^\nu = 4g^{\mu\nu}$$
This also implies:
$$\mathrm{Tr}\not{a}\not{b} = 4a\cdot b$$

4. ***Exercise 15*** Calculate $\mathrm{Tr}(\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma)$. Hint: Move γ^σ all the way to the left, using the anticommutation relations. Then use 3.

   Homework: Prove that $\mathrm{Tr}(\gamma^{\mu_1}\gamma^{\mu_2}\cdots\gamma^{\mu_{2n}})$ has $(2n-1)!!$ terms.

5. $\mathrm{Tr}(\gamma^5\gamma^{\mu_1}\gamma^{\mu_2}\cdots\gamma^{\mu_{2n+1}}) = 0$. This follows from 1. and from the fact that γ^5 consists of even number of γ's.

6. $\mathrm{Tr}\gamma^5 = \mathrm{Tr}(\gamma^0\gamma^0\gamma^5) = -\mathrm{Tr}(\gamma^0\gamma^5\gamma^0) = -\mathrm{Tr}\gamma^5 = 0$

7. $\mathrm{Tr}(\gamma^5\gamma^\mu\gamma^\nu) = 0$. (Same trick as above, with $\gamma^\alpha \neq \mu, \nu$ instead of γ^0.)

8. $\mathrm{Tr}(\gamma^5\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma) = -4i\epsilon^{\mu\nu\rho\sigma}$, with $\epsilon^{0123} = 1$. Careful: convention with $\epsilon^{0123} = -1$ is also in use.

Contraction identities

1. $$\gamma^\mu\gamma_\mu = \frac{1}{2}g_{\mu\nu}\underbrace{(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu)}_{2g^{\mu\nu}} = g_{\mu\nu}g^{\mu\nu} = 4$$

2. $$\gamma^\mu\underbrace{\gamma^\alpha\gamma_\mu}_{-\gamma_\mu\gamma^\alpha+2g^\alpha_\mu} = -4\gamma^\alpha + 2\gamma^\alpha = -2\gamma^\alpha$$

3. ***Exercise 16*** Contract $\gamma^\mu\gamma^\alpha\gamma^\beta\gamma_\mu$.

4. $\gamma^\mu\gamma^\alpha\gamma^\beta\gamma^\gamma\gamma_\mu = -2\gamma^\gamma\gamma^\beta\gamma^\alpha$

Exercise 17 Calculate traces in $\overline{|\mathcal{M}|^2}$:

$$\begin{aligned}\mathrm{Tr}[(\not{p}_1 + m_1)\gamma^\mu(\not{p}_2 - m_2)\gamma^\nu] &= ?\\ \mathrm{Tr}[(\not{p}_4 - m_4)\gamma_\mu(\not{p}_3 + m_3)\gamma_\nu] &= ?\end{aligned}$$

Exercise 18 Calculate $\overline{|\mathcal{M}|^2}$

6.4 Kinematics in the center-of-mass frame

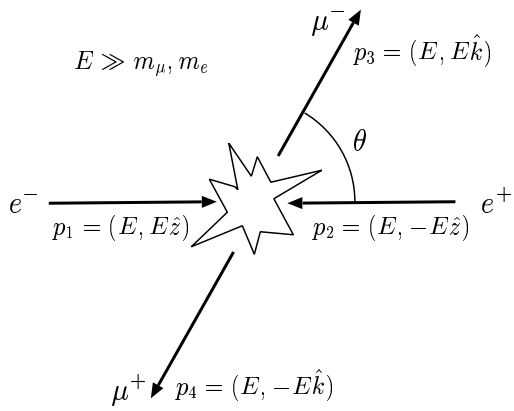
In e^+e^- coliders often $p_i \gg m_e, m_\mu$, $i = 1, \ldots, 4$, so we can take

$$m_i \to 0 \qquad \text{“high-energy” or “extreme relativistic” limit}$$

Then

$$\overline{|\mathcal{M}|^2} = \frac{8e^4}{(p_1+p_2)^4}[(p_1\cdot p_3)(p_2\cdot p_4) + (p_1\cdot p_4)(p_2\cdot p_3)] \tag{63}$$

To calculate scattering cross-section σ we have to specialize to some particular frame (σ is *not* frame-independent). For e^+e^- colliders the most relevant is the center-of-mass (CM) frame:



Exercise 19 Express $\overline{|\mathcal{M}|^2}$ in terms of E and θ.

6.5 Integration over two-particle phase space

Now we can use the “golden rule” (45) for the $1+2 \to 3+4$ differential scattering cross-section

$$d\sigma = \frac{1}{u_\alpha}\frac{1}{2E_1}\frac{1}{2E_2}\overline{|\mathcal{M}|^2}\, d\text{Lips}_2 \tag{64}$$

where two-particle phase space to be integrated over is

$$d\text{Lips}_2 = (2\pi)^4\delta^4(p_1+p_2-p_3-p_4)\frac{d^3p_3}{(2\pi)^3\,2E_3}\frac{d^3p_4}{(2\pi)^3\,2E_4}\ . \tag{65}$$

First we integrate over four out of six integration variables, and we do this in general frame. δ-function makes the integration over d^3p_4 trivial giving

$$d\text{Lips}_2 = \frac{1}{(2\pi)^2\, 4E_3E_4}\,\delta(E_1+E_2-E_3-E_4)\,\underbrace{d^3p_3}_{\boldsymbol{p}_3^2 d|\boldsymbol{p}_3|d\Omega_3} \tag{66}$$

Now we integrate over $d|\boldsymbol{p}_3|$ by noting that E_3 and E_4 are functions of $|\boldsymbol{p}_3|$

$$\begin{aligned} E_3 &= E_3(|\boldsymbol{p}_3|) = \sqrt{\boldsymbol{p}_3^2+m_3^2}\,, \\ E_4 &= \sqrt{\boldsymbol{p}_4^2+m_4^2} = \sqrt{\boldsymbol{p}_3^2+m_4^2}\,, \end{aligned}$$

and by δ-function relation

$$\delta(E_1+E_2-\sqrt{\boldsymbol{p}_3^2+m_3^2}-\sqrt{\boldsymbol{p}_3^2+m_4^2}) = \delta[f(|\boldsymbol{p}_3|)] = \frac{\delta(|\boldsymbol{p}_3|-|\boldsymbol{p}_3^{(0)}|)}{|f'(|\boldsymbol{p}_3|)|_{|\boldsymbol{p}_3|=|\boldsymbol{p}_3^{(0)}|}}\,. \tag{67}$$

Here $|\boldsymbol{p}_3|$ is just the integration variable and $|\boldsymbol{p}_3^{(0)}|$ is the zero of $f(|\boldsymbol{p}_3|)$ i.e. the *actual* momentum of the third particle. After we integrate over $d|\boldsymbol{p}_3|$ we put $|\boldsymbol{p}_3^{(0)}| \to |\boldsymbol{p}_3|$.

Since

$$f'(|\boldsymbol{p}_3|) = -\frac{E_3+E_4}{E_3E_4}|\boldsymbol{p}_3|\,, \tag{68}$$

we get

$$d\text{Lips}_2 = \frac{|\boldsymbol{p}_3|d\Omega}{16\pi^2(E_1+E_2)}\,. \tag{69}$$

Now we again specialize to the CM frame and note that the flux factor is

$$4E_1E_2u_\alpha = 4\sqrt{(p_1\cdot p_2)^2-m_1^2m_2^2} = 4|\boldsymbol{p}_1|(E_1+E_2)\,, \tag{70}$$

giving finally

$$\frac{d\sigma_{\text{CM}}}{d\Omega} = \frac{1}{64\pi^2(E_1+E_2)^2}\frac{|\boldsymbol{p}_3|}{|\boldsymbol{p}_1|}\overline{|\mathcal{M}|^2}\,. \tag{71}$$

Note that we kept masses in each step so this formula is generally valid for any CM scattering.

For our particular $e^-e^+ \to \mu^-\mu^+$ scattering this gives the final result for differential cross-section (introducing the fine structure constant $\alpha = e^2/(4\pi)$)

$$\frac{d\sigma}{d\Omega} = \frac{\alpha^2}{16E^2}(1+\cos^2\theta)\,. \tag{72}$$

Exercise 20 Integrate this to get the total cross section σ.

Note that it is obvious that $\sigma \propto \alpha^2$, and that dimensional analysis requires $\sigma \propto 1/E^2$, so only angular dependence $(1+\cos^2\theta)$ tests QED as a theory of leptons and photons.

6.6 Summary of steps

To recapitulate, calculating (unpolarized) scattering cross-section (or decay width) consists of the following steps:

1. drawing the Feynman diagram(s)
2. writing $-i\mathcal{M}$ using the Feynman rules
3. squaring $\mathcal{M}$ and using the Casimir trick to get traces
4. evaluating traces
5. applying kinematics of the chosen frame
6. integrating over the phase space

6.7 Mandelstam variables

Mandelstam variables s, t and u are often used in scattering calculations. They are defined (for $1 + 2 \to 3 + 4$ scattering) as

$$\begin{aligned} s &= (p_1 + p_2)^2 \\ t &= (p_1 - p_3)^2 \\ u &= (p_1 - p_4)^2 \end{aligned}$$

Exercise 21 Prove that $s + t + u = m_1^2 + m_2^2 + m_3^2 + m_4^2$

This means that only two Mandelstam variables are independent. Their main advantage is that they are Lorentz invariant which renders them convenient for Feynman amplitude calculations. Only at the end we can exchange them for "experimenter's" variables E and θ.

Exercise 22 Express $\overline{|\mathcal{M}|^2}$ for $e^-e^+ \to \mu^-\mu^+$ scattering in terms of Mandelstam variables.

Appendix: Doing Feynman diagrams on a computer

There are several computer programs that can perform some or all of the steps in the calculation of Feynman diagrams. Here is a simple session with one such program, `FeynCalc` [2] package for Wolfram's *Mathematica*, where we calculate the same process, $e^-e^+ \to \mu^-\mu^+$, that we just calculated in the text. Alternative framework, relying only on open source software is FORM [3].

FeynCalc demonstration

This *Mathematica* notebook demonstrates computer calculation of Feynman invariant amplitude for $e^- e^+ \to \mu^- \mu^+$ scattering, using Feyncalc package.

First we load FeynCalc into Mathematica

```
In[1]:= << HighEnergyPhysics`fc`
```

FeynCalc 4.1.0.3b Evaluate ?FeynCalc for help or visit www.feyncalc.org

Spin−averagedFeynman amplitude squared $\overline{|\mathcal{M}|^2}$ after using Feynman rules and applying the Casimir trick:

```
In[2]:= Msq = e^4/(4 (p1 + p2)^4) Contract[Tr[(GS[p1] + me).GA[μ].(GS[p2] - me).GA[ν]]
          Tr[(GS[p4] - mm).GA[μ].(GS[p3] + mm).GA[ν]]]
```

Out[2]= $\frac{1}{4\,(\mathrm{p1}+\mathrm{p2})^4}\left(e^4\left(64\,\mathrm{mm}^2\,\mathrm{me}^2 + 32\,\mathrm{p3}\cdot\mathrm{p4}\,\mathrm{me}^2 + 32\,\mathrm{mm}^2\,\mathrm{p1}\cdot\mathrm{p2} + 32\,\mathrm{p1}\cdot\mathrm{p4}\,\mathrm{p2}\cdot\mathrm{p3} + 32\,\mathrm{p1}\cdot\mathrm{p3}\,\mathrm{p2}\cdot\mathrm{p4}\right)\right)$

Traces were evaluated and contractions performed automatically. Now we introduce Mandelstam variables by substitution rules,

```
In[3]:= prod[a_, b_] := Pair[Momentum[a], Momentum[b]];
        mandelstam = {prod[p1, p2] → (s - me^2 - me^2) / 2, prod[p3, p4] → (s - mm^2 - mm^2) / 2,
           prod[p1, p3] → (t - me^2 - mm^2) / 2, prod[p2, p4] → (t - me^2 - mm^2) / 2,
           prod[p1, p4] → (u - me^2 - mm^2) / 2, prod[p2, p3] → (u - me^2 - mm^2) / 2, (p1 + p2) → Sqrt[s]};
```

and apply these substitutions to our amplitude:

```
In[5]:= Msq /. mandelstam
```

Out[5]= $\frac{1}{4\,s^2}\left(e^4\left(64\,\mathrm{mm}^2\,\mathrm{me}^2 + 16\,(s-2\,\mathrm{mm}^2)\,\mathrm{me}^2 + 8\,(-\mathrm{me}^2-\mathrm{mm}^2+t)^2 + 8\,(-\mathrm{me}^2-\mathrm{mm}^2+u)^2 + 16\,\mathrm{mm}^2\,(s-2\,\mathrm{me}^2)\right)\right)$

This result can be simplified by eliminating one Mandelstam variable:

```
In[6]:= Simplify[TrickMandelstam[%, s, t, u, 2 me^2 + 2 mm^2]]
```

Out[6]= $\frac{2\,e^4\,(2\,\mathrm{me}^4 + 4\,(\mathrm{mm}^2-u)\,\mathrm{me}^2 + 2\,\mathrm{mm}^4 + s^2 + 2\,u^2 - 4\,\mathrm{mm}^2\,u + 2\,s\,u)}{s^2}$

If we go to ultra−relativistic limit, we get result in agreement with our hand calculation:

```
In[7]:= Simplify[%% /. {mm → 0, me → 0}]
```

Out[7]= $\frac{2\,e^4\,(t^2+u^2)}{s^2}$

References

[1] D. Griffiths, *Introduction to elementary particles*, Wiley (1987)

[2] V. Shtabovenko, R. Mertig and F. Orellana, *New Developments in FeynCalc 9.0*, arXiv:1601.01167 [hep-ph].

[3] J. A. M. Vermaseren, *New features of FORM*, math-ph/0010025.

Quantization of the Free Electromagnetic Field: Photons and Operators

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Summary

The main ideas and equations for quantized free electromagnetic fields are developed and summarized here, based on the quantization procedure for coordinates (components of the vector potential $\mathbf{A}$) and their canonically conjugate momenta (components of the electric field $\mathbf{E}$). Expressions for $\mathbf{A}$, $\mathbf{E}$ and magnetic field $\mathbf{B}$ are given in terms of the creation and annihilation operators for the fields. Some ideas are proposed for the interpretation of photons at different polarizations: linear and circular. Absorption, emission and stimulated emission are also discussed.

1 Electromagnetic Fields and Quantum Mechanics

Here electromagnetic fields are considered to be quantum objects. It's an interesting subject, and the basis for consideration of interactions of particles with EM fields (light). Quantum theory for light is especially important at low light levels, where the number of light quanta (or photons) is small, and the fields cannot be considered to be continuous (opposite of the classical limit, of course!).

Here I follow the traditinal approach of quantization, which is to identify the coordinates and their conjugate momenta. Once that is done, the task is straightforward. Starting from the classical mechanics for Maxwell's equations, the fundamental coordinates and their momenta in the QM system must have a commutator defined analogous to $[x, p_x] = i\hbar$ as in any simple QM system. This gives the correct scale to the quantum fluctuations in the fields and any other dervied quantities. The creation and annihilation operators will have a unit commutator, $[a, a\dagger] = 1$, but they have to be connected to the fields correctly. I try to show how these relations work. Getting the correct normalization on everything is important when interactions of the EM fields with matter are considered.

It is shown that the quantized fields are nothing more than a system of decoupled harmonic oscillators, at a collection of different wavevectors and wave-polarizations. The knowledge of how to quantize simple harmonic oscillators greatly simplifies the EM field problem. In the end, we get to see how the basic quanta of the EM fields, which are called photons, are created and annihilated in discrete processes of emission and absorption by atoms or matter in general. I also want to discuss different aspects of the photons, such as their polarization, transition rules, and conservation laws.

Later in related notes I'll talk about how this relates to describing two other topics of interest: quantum description of the dielectric response of materials (dielectric function $\epsilon(\omega)$), and, effects involving circularly polarized light incident on a material in the presence of a DC magnetic field (Faraday effect). I want to describe especially the quantum theory for the Faraday effect, which is the rotation of the polarization of linearly polarized light when it passes through a medium in a DC magnetic field parallel to the light rays. That is connected to the dielectric function, hence the interest in these related topics.

1.1 Maxwell's equations and Lagrangian and Hamiltonian Densities

A Lagrangian density for the free EM field is

$$\mathcal{L} = \frac{1}{8\pi}\left[\mathbf{E}^2 - \mathbf{B}^2\right] \tag{1}$$

[It's integral over time and space will give the classical **action** for a situation with electromagnetic fields.] This may not be too obvious, but I take it as an excercise for the reader in classical mechanics, because here we want to get to the quantum problem. Maxwell's equations in free space, written for the electric ($\mathbf{E}$) and magnetic ($\mathbf{B}$) fields in CGS units, are

$$\nabla \cdot \mathbf{B} = 0, \qquad \nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = 0, \qquad \nabla \cdot \mathbf{E} = 0, \qquad \nabla \times \mathbf{B} - \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} = 0 \tag{2}$$

The zero divegence of $\mathbf{B}$ and Faraday's Law (1st and 2nd eqns) allow the introduction of vector and scalar potentials, $\mathbf{A}$ and Φ, respectively, that give the fields,

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \mathbf{E} = -\nabla\Phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} \tag{3}$$

I consider a problem far from sources. If sources were present, they would appear in the last two equations in (2), so these same potentials could still apply. The potentials are not unique and have a gauge symmetry. They can be shifted using some guage transformation (f) without changing the electric and magnetic fields:

$$\mathbf{A}' = \mathbf{A} + \nabla f, \qquad \Phi' = \Phi - \frac{1}{c}\frac{\partial f}{\partial t} \tag{4}$$

The Euler-Lagrange variation of the Lagrangian w.r.t the **coordinates** $q = (\Phi, A_x, A_y, A_z)$ gives back Maxwell's equations. Recall Euler-Lagrange equation and try it as a practice problem in classical mechanics.

To approach quantization, the canonical momenta p_i need to be identified. But there is no time derivative of Φ in $\mathcal{L}$, so there is no p_Φ and Φ should be eliminated as a coordinate, in some sense. There *are* time derivatives of $\mathbf{A}$, hence their canonical momenta are found as

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{A}_i} = \frac{1}{4\pi c}\left(\frac{\partial \Phi}{\partial x_i} + \frac{1}{c}\frac{\partial A_i}{\partial t}\right) = -\frac{1}{4\pi c}E_i, \quad i = 1, 2, 3 \tag{5}$$

The transformation to the Hamiltonian energy density is the Legendre transform,

$$\mathcal{H} = \sum_i p_i \dot{q}_i - \mathcal{L} = \mathbf{p} \cdot \frac{\partial \mathbf{A}}{\partial t} - \mathcal{L} = 2\pi c^2 \mathbf{p}^{\,2} + \frac{1}{8\pi}\left(\nabla \times A\right)^2 - c\mathbf{p} \cdot \nabla\Phi \tag{6}$$

When integrated over all space, the last term gives nothing, because $\nabla \cdot \mathbf{E} = 0$, and the first two terms give a well known result for the effective energy density, in terms of the EM fields,

$$\mathcal{H} = \frac{1}{8\pi}\left(\mathbf{E}^2 + \mathbf{B}^2\right) \tag{7}$$

We might keep the actual Hamiltonian in terms of the coordinates $\mathbf{A}$ and their conjugate momenta $\mathbf{p}$, leading to the classical EM energy,

$$H = \int d^3r \left[2\pi c^2 \mathbf{p}^{\,2} + \frac{1}{8\pi}\left(\nabla \times \mathbf{A}\right)^2\right] \tag{8}$$

Now it is usual to apply the **Coulomb gauge**, where $\Phi = 0$ and $\nabla \cdot \mathbf{A} = 0$. For one, this insures having just three coordinates and their momenta, so the mechanics is consistent. Also that is consistent with the fields needing three coordinates because they are three-dimensional fields. (We don't need six coordinates, because $\mathbf{E}$ and $\mathbf{B}$ are not independent. In a vague sense, the magnetic and electric fields have some mutual conjugate relationship.) We can use either the Lagrangian or Hamiltonian equations of motion to see the dynamics. For instance, by the Hamiltonian method, we have

$$\dot{q}_i = \frac{\delta \mathcal{H}}{\delta p_i}, \qquad \dot{p}_i = -\frac{\delta \mathcal{H}}{\delta q_i} \tag{9}$$

Recall that the variation of a density like this means

$$\frac{\delta \mathcal{H}}{\delta f} \equiv \frac{\partial \mathcal{H}}{\partial f} - \sum_i \frac{\partial}{\partial x_i}\frac{\partial \mathcal{H}}{\partial\left(\frac{\partial f}{\partial x_i}\right)} - \frac{\partial}{\partial t}\frac{\partial \mathcal{H}}{\partial\left(\frac{\partial f}{\partial t}\right)} \tag{10}$$

The variation for example w.r.t coordinate $q_i = A_x$ gives the results

$$\frac{\partial A_x}{\partial t} = 4\pi c^2 p_x, \qquad \frac{\partial p_x}{\partial t} = \frac{1}{4\pi}\nabla^2 A_x \tag{11}$$

By combining these, we see that all the components of the vector potential (and the conjugate momentum, which is proportional to $\mathbf{E}$) satisfy a wave equation, as could be expected!

$$\nabla^2 \mathbf{A} - \frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} = 0 \tag{12}$$

Wave motion is essentially oscillatory, hence the strong connection of this problem to the harmonic oscillator solutions.

The above wave equation has plane wave solutions $e^{i\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t}$ at angular frequency $\omega_{\mathbf{k}}$ and wave vector $\mathbf{k}$ that have a linear dispersion relation, $\omega_{\mathbf{k}} = ck$. For the total field in some volume V, we can try a Fourier expansion over a collection of these modes, supposing periodic boundary conditions.

$$\mathbf{A}(\mathbf{r}, t) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} \mathbf{A}_{\mathbf{k}}(t)\ e^{i\mathbf{k}\cdot\mathbf{r}} \tag{13}$$

Each coefficient $\mathbf{A}_{\mathbf{k}}(t)$ is an amplitude for a wave at the stated wave vector. The different modes are orthogonal (or independent), due to the normalization condition

$$\int d^3\mathbf{r}\ e^{i\mathbf{k}\cdot\mathbf{r}}\ e^{-i\mathbf{k}'\cdot\mathbf{r}} = V\delta_{\mathbf{k}\mathbf{k}'} \tag{14}$$

The gauge assumption $\nabla\cdot\mathbf{k} = 0$ then is the same as $\mathbf{k}\cdot\mathbf{A}_{\mathbf{k}} = 0$, which shows that the waves are transverse. For any $\mathbf{k}$, there are two transverse directions, and hence, two independent polarizations directions, identified by unit vectors $\mathbf{e}_{\mathbf{k}\alpha}$, $\alpha = 1, 2$. Thus the total amplitude looks like

$$\mathbf{A}_{\mathbf{k}} = \hat{\epsilon}_{\mathbf{k}1}A_{\mathbf{k}1} + \hat{\epsilon}_{\mathbf{k}2}A_{\mathbf{k}2} = \sum_{\alpha}\hat{\epsilon}_{\mathbf{k}\alpha}A_{\mathbf{k}\alpha} \tag{15}$$

Yet, from the wave equation, both polarizations are found to oscillate identically, except perhaps not in phase,

$$\mathbf{A}_{\mathbf{k}}(t) = \mathbf{A}_{\mathbf{k}}\ e^{-i\omega_{\mathbf{k}}t} \tag{16}$$

Now the amplitudes $\mathbf{A}_{\mathbf{k}}$ are generally complex, whereas, we want to have the actual field being quantized to be real. This can be accomplished by combining these waves appropriately with their complex conjugates. For example, the simple waves $A = \cos kx = (e^{ikx} + e^{-ikx})/2$ and $A = \sin kx = (e^{ikx} - e^{-ikx})/2i$ are sums of "positive" and "negative" wavevectors with particular amplitudes. Try to write $\mathbf{A}$ in (13) in a different way that exhibits the positive and negative wavevectors together,

$$\mathbf{A}(\mathbf{r}, t) = \frac{1}{2\sqrt{V}}\sum_{\mathbf{k}}\left[\mathbf{A}_{\mathbf{k}}(t)\ e^{i\mathbf{k}\cdot\mathbf{r}} + \mathbf{A}_{-\mathbf{k}}(t)\ e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{17}$$

[The sum over $\mathbf{k}$ here includes wave vectors in all directions. Then both $\mathbf{k}$ and $-\mathbf{k}$ are included twice. It is divided by 2 to avoid double counting.] In order for this to be real, a little consideration shows that the 2nd term must be the c.c. of the first term,

$$\mathbf{A}_{-\mathbf{k}} = \mathbf{A}_{\mathbf{k}}{}^* \tag{18}$$

A wave needs to identified by both $\mathbf{A}_{\mathbf{k}}$ and its complex conjugate (or equivalently, two real constants). So the vector potential is written in Fourier space as

$$\mathbf{A}(\mathbf{r}, t) = \frac{1}{2\sqrt{V}}\sum_{\mathbf{k}}\left[\mathbf{A}_{\mathbf{k}}(t)\ e^{i\mathbf{k}\cdot\mathbf{r}} + \mathbf{A}^*_{\mathbf{k}}(t)\ e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{19}$$

Note that the c.c. reverses the sign on the frequency also, so the first term oscillates at positive frequency and the second at negative frequency. But curiously, both together give a real wave

traveling along the direction of $\mathbf{k}$. Based on this expression, the fields are easily determined by applying (3), with $\nabla \to \pm i\mathbf{k}$,

$$\mathbf{E}(\mathbf{r},t) = \frac{i}{2c\sqrt{V}} \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left[\mathbf{A}_{\mathbf{k}}(t)\ e^{i\mathbf{k}\cdot\mathbf{r}} - \mathbf{A}_{\mathbf{k}}^{*}(t)\ e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \tag{20}$$

$$\mathbf{B}(\mathbf{r},t) = \frac{i}{2\sqrt{V}} \sum_{\mathbf{k}} \mathbf{k}\times \left[\mathbf{A}_{\mathbf{k}}(t)\ e^{i\mathbf{k}\cdot\mathbf{r}} - \mathbf{A}_{\mathbf{k}}^{*}(t)\ e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \tag{21}$$

Now look at the total energy, i.e., evaluate the Hamiltonian. It should be easy because of the orthogonality of the plane waves, assumed normalized in a box of volume V. We also know that $\mathbf{k}$ is perpendicular to $\mathbf{A}$ (transverse waves!) which simplifies the magnetic energy. Still, some care is needed in squaring the fields and integrating. There are direct terms (btwn $\mathbf{k}$ and itself) and indirect terms (btwn $\mathbf{k}$ and $-\mathbf{k}$).

$$\int d^3\mathbf{r}\ |\mathbf{E}|^2 = \frac{1}{4c^2V} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \omega_{\mathbf{k}}\omega_{\mathbf{k}'} \int d^3\mathbf{r}\ \left[\mathbf{A}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} - \mathbf{A}_{\mathbf{k}}^{*} e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \left[\mathbf{A}_{\mathbf{k}'}^{*} e^{-i\mathbf{k}'\cdot\mathbf{r}} - \mathbf{A}_{\mathbf{k}'} e^{i\mathbf{k}'\cdot\mathbf{r}} \right] \tag{22}$$

Upon integration over the volume, the orthogonality relation will give 2 terms with $\mathbf{k}' = \mathbf{k}$ and 2 terms with $\mathbf{k}' = -\mathbf{k}$, for 4 equivalent terms in all. The same happens for the calculation of the magnetic energy. Also one can't forget that $\mathbf{A}_{\mathbf{k}}$ is the same as $\mathbf{A}_{-\mathbf{k}}^{*}$. These become

$$\frac{1}{8\pi} \int d^3\mathbf{r}\ |\mathbf{E}|^2 = \frac{1}{8\pi} \sum_{\mathbf{k}} \frac{\omega_{\mathbf{k}}^2}{c^2} |\mathbf{A}_{\mathbf{k}}(t)|^2 \tag{23}$$

$$\frac{1}{8\pi} \int d^3\mathbf{r}\ |\mathbf{B}|^2 = \frac{1}{8\pi} \sum_{\mathbf{k}} \mathbf{k}^2 |\mathbf{A}_{\mathbf{k}}(t)|^2 \tag{24}$$

Of course, $\mathbf{k}^2$ in the expression for magnetic energy is the same as $\omega_{\mathbf{k}}^2/c^2$ in that for electric energy. Then it is obvious that the magnetic and electric energies are equal. The net total energy is simple,

$$H = \frac{1}{8\pi} \int d^3\mathbf{r}\ \left(|\mathbf{E}|^2 + |\mathbf{B}|^2 \right) = \frac{1}{8\pi} \sum_{\mathbf{k}} k^2 |\mathbf{A}_{\mathbf{k}}|^2 = \frac{1}{4\pi} \sum_{\mathbf{k}\alpha} k^2 |A_{\mathbf{k}\alpha}|^2 \tag{25}$$

The last form recalls that each wave vector is associated with two independent polarizations. They are orthogonal, so there are no cross terms between them from squaring.

The Hamiltonian shows that the modes don't interfere with each other, imagine how it is possible that EM fields in vacuum can be completely linear! But this is good because now we just need to quantize the modes as if they are a collection of independent harmonic oscillators. To do that, need to transform the expression into the language of the coordinates and conjugate momenta. It would be good to see H expressed through squared coordinate (potential energy term) and squared momentem (kinetic energy term).

The electric field is proportional to the canonical momentum, $\mathbf{E} = -4\pi c\mathbf{p}$. So really, the electric field energy term already looks like a sum of squared momenta. Similarly, the magnetic field is determined by the curl of the vector potential, which is the basic coordinate here. So we have some relations,

$$\mathbf{p}(\mathbf{r},t) = -\frac{1}{4\pi c}\mathbf{E} = \frac{-i}{8\pi c^2\sqrt{V}} \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left[\mathbf{A}_{\mathbf{k}}(t)\ e^{i\mathbf{k}\cdot\mathbf{r}} - \mathbf{A}_{\mathbf{k}}^{*}(t)\ e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \tag{26}$$

This suggests the introduction of the momenta at each wavevector, i.e., analogous with the Fourier expansion for the vector potential (i.e., the generalized coordinates),

$$\mathbf{p}(\mathbf{r},t) = \frac{1}{2\sqrt{V}} \sum_{\mathbf{k}} \left[\mathbf{p}_{\mathbf{k}}(t)\ e^{i\mathbf{k}\cdot\mathbf{r}} + \mathbf{p}_{\mathbf{k}}^{*}(t)\ e^{-i\mathbf{k}\cdot\mathbf{r}} \right] \tag{27}$$

Then we can make the important identifications,

$$\mathbf{p}_{\mathbf{k}}(t) = \frac{-i\omega_{\mathbf{k}}}{4\pi c^2} \mathbf{A}_{\mathbf{k}}(t) \tag{28}$$

Even more simply, just write the electric field (and its energy) in terms of the momenta now.

$$\mathbf{E}(\mathbf{r},t) = -4\pi c\mathbf{p}(\mathbf{r},t) = \frac{-2\pi c}{\sqrt{V}}\sum_{\mathbf{k}}\left[\mathbf{p}_{\mathbf{k}}(t)e^{i\mathbf{k}\cdot\mathbf{r}} + \mathbf{p}^*_{\mathbf{k}}(t)e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{29}$$

When squared, the electric energy involves four equivalent terms, and there results

$$\frac{1}{8\pi}\int d^3\mathbf{r}\ |\mathbf{E}|^2 = \frac{16\pi^2c^2}{8\pi}\sum_{\mathbf{k}}\mathbf{p}_{\mathbf{k}}\cdot\mathbf{p}^*_{\mathbf{k}} = 2\pi c^2\sum_{\mathbf{k}}\mathbf{p}_{\mathbf{k}}\cdot\mathbf{p}^*_{\mathbf{k}} \tag{30}$$

Also rewrite the magnetic energy. The generalized coordinates are the components of $\mathbf{A}$, i.e., let's write

$$\mathbf{q}_{\mathbf{k}} = \mathbf{A}_{\mathbf{k}} \tag{31}$$

Consider the magnetic field written this way,

$$\mathbf{B}(\mathbf{r},t) = \frac{i}{2\sqrt{V}}\sum_{\mathbf{k}}\mathbf{k}\times\left[\mathbf{q}_{\mathbf{k}}(t)\ e^{i\mathbf{k}\cdot\mathbf{r}} - \mathbf{q}^*_{\mathbf{k}}(t)\ e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{32}$$

and the associated energy is written,

$$\frac{1}{8\pi}\int d^3\mathbf{r}\ |\mathbf{B}|^2 = \frac{4}{4\times 8\pi}\sum_{\mathbf{k}}\mathbf{k}^2\mathbf{q}_{\mathbf{k}}\cdot\mathbf{q}^*_{\mathbf{k}} = \frac{1}{8\pi c^2}\sum_{\mathbf{k}}\omega^2_{\mathbf{k}}\mathbf{q}_{\mathbf{k}}\cdot\mathbf{q}^*_{\mathbf{k}} \tag{33}$$

This gives the total canonical Hamiltonian, expressed in the Fourier modes, as

$$H = 2\pi c^2\sum_{\mathbf{k}}\mathbf{p}_{\mathbf{k}}\cdot\mathbf{p}^*_{\mathbf{k}} + \frac{1}{8\pi c^2}\sum_{\mathbf{k}}\omega^2_{\mathbf{k}}\mathbf{q}_{\mathbf{k}}\cdot\mathbf{q}^*_{\mathbf{k}} \tag{34}$$

Check that it works for the classical problem. To apply correctly, one has to keep in mind that at each mode $\mathbf{k}$, there are the *two amplitudes*, $\mathbf{q}_{\mathbf{k}}$ and $\mathbf{q}^*_{\mathbf{k}}$. In addition, it is important to remember that the sum goes over all positive and negative $\mathbf{k}$, and that $\mathbf{q}_{-\mathbf{k}}$ is the same as $\mathbf{q}^*_{\mathbf{k}}$.

Curiously, look what happens if you think that the Hamiltonian has only real coordinates, and write incorrectly

$$H_{\text{oo}} = \sum_{\mathbf{k}}\left[2\pi c^2\mathbf{p}^{\mathbf{2}}_{\mathbf{k}} + \frac{\omega^2_{\mathbf{k}}}{8\pi c^2}\mathbf{q}^{\mathbf{2}}_{\mathbf{k}}\right] \tag{35}$$

The Hamilton equations of motion become

$$\dot{\mathbf{p}}_{\mathbf{k}} = \frac{\delta H_{\text{oo}}}{\delta\mathbf{q}_{\mathbf{k}}} = \frac{\omega^2_{\mathbf{k}}}{4\pi c^2}\ \mathbf{q}_{\mathbf{k}}, \qquad \dot{\mathbf{q}}_{\mathbf{k}} = -\frac{\delta H_{\text{oo}}}{\delta\mathbf{p}_{\mathbf{k}}} = -4\pi c^2\ \mathbf{p}_{\mathbf{k}} \tag{36}$$

Combining these actually leads to the correct frequency of oscillation, but only by luck!

$$\ddot{\mathbf{p}}_{\mathbf{k}} = \frac{\omega^2_{\mathbf{k}}}{4\pi c^2}\ \dot{\mathbf{q}}_{\mathbf{k}} = -\omega^2_{\mathbf{k}}\ \mathbf{p}_{\mathbf{k}}, \qquad \ddot{\mathbf{q}}_{\mathbf{k}} = -4\pi c^2\ \dot{\mathbf{p}}_{\mathbf{k}} = -\omega^2_{\mathbf{k}}\ \mathbf{q}_{\mathbf{k}} \tag{37}$$

These are oscillating at frequency $\omega_{\mathbf{k}}$.

Now do the math (more) correctly. Variation of Hamiltonian (34) w.r.t. $\mathbf{q}_{\mathbf{k}}$ and $\mathbf{q}^*_{\mathbf{k}}$ are different things. On the other hand, $\mathbf{q}_{\mathbf{k}}$ and $\mathbf{q}^*_{-\mathbf{k}}$ are the same, so don't forget to account for that. It means that a term at negative wave vector is just like the one at positive wave vector: $\mathbf{q}_{-\mathbf{k}}\mathbf{q}^*_{-\mathbf{k}} = \mathbf{q}^*_{\mathbf{k}}\mathbf{q}_{\mathbf{k}}$. This doubles the interaction. The variations found are

$$\dot{\mathbf{p}}_{\mathbf{k}} = \frac{\delta H}{\delta\mathbf{q}_{\mathbf{k}}} = \frac{\omega^2_{\mathbf{k}}}{4\pi c^2}\ \mathbf{q}^*_{\mathbf{k}}, \qquad \dot{\mathbf{q}}_{\mathbf{k}} = -\frac{\delta H}{\delta\mathbf{p}_{\mathbf{k}}} = -4\pi c^2\ \mathbf{p}^*_{\mathbf{k}} \tag{38}$$

$$\dot{\mathbf{p}}^*_{\mathbf{k}} = \frac{\delta H}{\delta\mathbf{q}^*_{\mathbf{k}}} = \frac{\omega^2_{\mathbf{k}}}{4\pi c^2}\ \mathbf{q}_{\mathbf{k}}, \qquad \dot{\mathbf{q}}^*_{\mathbf{k}} = -\frac{\delta H}{\delta\mathbf{p}^*_{\mathbf{k}}} = -4\pi c^2\ \mathbf{p}_{\mathbf{k}} \tag{39}$$

Now we can see that the correct frequency results, all oscillate at $\omega_{\mathbf{k}}$. For example,

$$\ddot{\mathbf{p}}_{\mathbf{k}} = \frac{\omega^2_{\mathbf{k}}}{4\pi c^2}\ \dot{\mathbf{q}}^*_{\mathbf{k}} = -\omega^2_{\mathbf{k}}\mathbf{p}_{\mathbf{k}} \qquad \ddot{\mathbf{q}}_{\mathbf{k}} = -4\pi c^2\ \dot{\mathbf{p}}^*_{\mathbf{k}} = -\omega^2_{\mathbf{k}}\mathbf{q}_{\mathbf{k}} \tag{40}$$

There are tricky steps in how to do the algebra correctly. Once worked through, we find that the basic modes oscillate at the frequency required by the light wave dispersion relation, $\omega_{\mathbf{k}} = ck$.

1.2 Quantization of modes: Simple harmonic oscillator example

Next the quantization of each mode needs to be accomplished. But since each mode analogous to a harmonic oscillator, as we'll show, the quantization is not too difficult. We already can see that the modes are independent. So proceed essentially on the individual modes, at a given wave vector and polarization. But I won't for now be writing any polarization indices, for simplicity.

Recall the quantization of a simple harmonic oscillator. The Hamiltonian can be re-expressed in some rescaled operators:

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 = \frac{\hbar\omega}{2}\left(P^2 + Q^2\right); \qquad Q = \sqrt{\frac{m\omega}{\hbar}}q, \;\; P = \frac{1}{\sqrt{m\hbar\omega}}p \tag{41}$$

Then if the original commutator is $[x, p] = i\hbar$, we have a unit commutator here,

$$[Q, P] = \sqrt{\frac{m\omega}{\hbar}}\frac{1}{\sqrt{m\hbar\omega}}[x, p] = i \tag{42}$$

The Hamiltonian can be expressed in a symmetrized form as follows:

$$H = \frac{\hbar\omega}{2}\frac{1}{2}\left[(Q + iP)(Q - iP) + (Q - iP)(Q + iP)\right] \tag{43}$$

This suggest defining the annihilation and creation operators

$$a = \frac{1}{\sqrt{2}}(Q + iP), \qquad a^\dagger = \frac{1}{\sqrt{2}}(Q - iP) \tag{44}$$

Their commutation relation is then conveniently unity,

$$[a, a^\dagger] = (\frac{1}{\sqrt{2}})^2[Q + iP, Q - iP] = \frac{1}{2}\left\{-i[Q, P] + i[P, Q]\right\} = 1 \tag{45}$$

The coordinate and momentum are expressed

$$Q = \frac{1}{\sqrt{2}}(a + a^\dagger), \qquad P = \frac{1}{i\sqrt{2}}(a - a^\dagger). \tag{46}$$

The Hamiltonian becomes

$$H = \frac{\hbar\omega}{2}(aa^\dagger + a^\dagger a) = \hbar\omega(a^\dagger a + \frac{1}{2}) \tag{47}$$

where the last step used the commutation relation in the form, $aa^\dagger = a^\dagger a + 1$. The operator $\hat{n} = a^\dagger a$ is the number operator that counts the quanta of excitation. The number operator can be easily shown to have the following commutation relations:

$$[n, a] = [a^\dagger a, a] = [a^\dagger, a]a = -a, \qquad [n, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger[a, a^\dagger] = +a, \tag{48}$$

These show that $a^\dagger$ creates or adds one quantum of excitation to the system, while a destroys or removes one quantum. The Hamiltonian famously shows how the system has a zero-point energy of $\hbar\omega/2$ and each quantum of excitation adds an additional $\hbar\omega$ of energy.

The eigenstates of the number operator $\hat{n} = a^\dagger a$ are also eigenstates of H. And while a and $a^\dagger$ lower and raise the number of quanta present, the eigenstates of the Hamiltonian are not their eigenstates. But later we need some matrix elements, hence it is good to summarize here exactly the operations of a or $a^\dagger$ on the number eigenstates, $|n\rangle$, which are assumed to be unit normalized.

If a state $|n\rangle$ is a normalized eigenstate of $\hat{n}$, with eigenvalue n, then we must have

$$a^\dagger|n\rangle = c_n|n + 1\rangle, \qquad \langle n|a = c_n^*\langle n + 1| \tag{49}$$

where c_n is a normalization constant. Putting these together, and using the commutation relation, gives

$$1 = \langle n|aa^\dagger|n\rangle = |c_n|^2\langle n + 1|n + 1\rangle \Longrightarrow |c_n|^2 = \langle n|aa^\dagger|n\rangle = \langle n|a^\dagger a + 1|n\rangle = n + 1 \tag{50}$$

In the same fashion, consider the action of the lowering operator,

$$a|n\rangle = d_n|n-1\rangle, \qquad \langle n|a^\dagger = d_n^*\langle n-1| \tag{51}$$

$$1 = \langle n|a^\dagger a|n\rangle = |d_n|^2\langle n-1|n-1\rangle \Longrightarrow |d_n|^2 = \langle n|a^\dagger a|n\rangle = n \tag{52}$$

Therefore when these operators act, they change the normalization slightly, and we can write

$$a^\dagger|n\rangle = \sqrt{n+1}\ |n+1\rangle, \qquad a|n\rangle = \sqrt{n}\ |n-1\rangle. \tag{53}$$

Indeed, the first of these can be iterated on the ground state $|0\rangle$ that has no quanta, to produce any excited state:

$$|n\rangle = \frac{1}{\sqrt{n!}}\,(a^\dagger)^n|0\rangle \tag{54}$$

Based on these relations, then it is easy to see the basic matrix elements,

$$\langle n+1|a^\dagger|n\rangle = \sqrt{n+1}, \qquad \langle n-1|a|n\rangle = \sqrt{n}. \tag{55}$$

An easy way to remember these, is that the factor in the square root is always the larger of the number of quanta in either initial or final states. These will be applied later.

1.3 Fundamental commutation relations for the EM modes

Now how to relate what we know to the EM field Hamiltonian, Eqn. (34)? The main difference there is the presence of operators together with their complex conjugates in the classical Hamiltonian. How to decide their fundamental commutators? That is based on the fundamental commutation relation in real space (for one component only):

$$[A_i(\mathbf{r},t), p_i(\mathbf{r}',t)] = i\hbar\ \delta(\mathbf{r}-\mathbf{r}'). \tag{56}$$

The fields are expressed as in Eqns. (19) and (27). Using these expressions to evaluate the LHS of (56),

$$[A_i(\mathbf{r},t), p_i(\mathbf{r}',t)] = \frac{1}{4V}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\left[\mathbf{A}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}} + \mathbf{A}^*_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}, \mathbf{p}_{\mathbf{k}'}e^{i\mathbf{k}'\cdot\mathbf{r}'} + \mathbf{p}^*_{\mathbf{k}'}e^{-i\mathbf{k}'\cdot\mathbf{r}'}\right] \tag{57}$$

In a finite volume, however, the following is a representation of a delta function:

$$\delta(\mathbf{r}-\mathbf{r}') = \frac{1}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \tag{58}$$

Although not a proof, we can see that (56) and (57) match if the mode operators have the following commutation relations (for each component):

$$[\mathbf{A}_{\mathbf{k}}, \mathbf{p}^*_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},\mathbf{k}'}, \quad [\mathbf{A}^*_{\mathbf{k}}, \mathbf{p}_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},\mathbf{k}'}, \quad [\mathbf{A}_{\mathbf{k}}, \mathbf{p}_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},-\mathbf{k}'}, \quad [\mathbf{A}^*_{\mathbf{k}}, \mathbf{p}^*_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},-\mathbf{k}'}. \tag{59}$$

These together with the delta function representation, give the result for the RHS of (57),

$$[A_i(\mathbf{r},t), p_i(\mathbf{r}',t)] = \frac{1}{4V}\sum_{\pm\mathbf{k}} i\hbar\left[2e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} + 2e^{i-\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\right] = i\hbar\ \delta(\mathbf{r}-\mathbf{r}'). \tag{60}$$

Thus the basic commutators of the modes are those in (59). Now we can apply them to quantize the EM fields.

1.4 The quantization of the EM fields

At some point, one should keep in mind that these canonical coordinates are effectively scalars, once the polarization is accounted for:

$$\mathbf{q}_{\mathbf{k}} = \sum_{\alpha} \hat{\epsilon}_k q_{\mathbf{k}\alpha}, \qquad \mathbf{p}_{\mathbf{k}} = \sum_{\alpha} \hat{\epsilon}_k p_{\mathbf{k}\alpha}. \tag{61}$$

The polarizations are decoupled, so mostly its effects can be ignored. But then the Hamiltonian (34) really has two terms at each wavevector, one for each polarization. For simplicity I will not be writing the polarization index, but just write scalar $q_{\mathbf{k}}$ and $p_{\mathbf{k}}$ for each mode's coordinate and momentum. For any scalar coordinate and its momentum, we postulate from (59)

$$[q_{\mathbf{k}}, p^\dagger_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},\mathbf{k}'}, \quad [q^\dagger_{\mathbf{k}}, p_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},\mathbf{k}'}, \quad [q_{\mathbf{k}}, p_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},-\mathbf{k}'}, \quad [q^\dagger_{\mathbf{k}}, p^\dagger_{\mathbf{k}'}] = i\hbar\delta_{\mathbf{k},-\mathbf{k}'}, \tag{62}$$

Note that the first two look to be inconsistent if you think of the adjoint operation as just complex conjugate. But they are correct. Noting that $(AB^\dagger)^\dagger = BA^\dagger$, we have

$$[A, B^\dagger]^\dagger = BA^\dagger - A^\dagger B = [B, A^\dagger] = -[A^\dagger, B] \tag{63}$$

Then applied to the problem with $A = q_{\mathbf{k}}$ and $B = p_{\mathbf{k}'}$

$$[q^\dagger_{\mathbf{k}}, p_{\mathbf{k}'}] = -[q_{\mathbf{k}}, p^\dagger_{\mathbf{k}'}]^\dagger = -(i\hbar\delta_{\mathbf{k},\mathbf{k}'})^\dagger = i\hbar\delta_{\mathbf{k},\mathbf{k}'} \tag{64}$$

So although the relations look unsual, they are correct.

Let's look at some algebra that hopefully leads to creation and annihilation operators. First, get some coordinates and momenta with unit normalized commutators. Suppose that a given mode $\mathbf{k}\alpha$ has a Hamiltonian from (34). Consider first one term at one wave vector: [Even though, classically, the terms at $\mathbf{k}$ and $-\mathbf{k}$ in the sum give equal contributions] Consider making a transformation to $Q_{\mathbf{k}}$ and $P_{\mathbf{k}}$,

$$H_{+\mathbf{k}\alpha} = 2\pi c^2 p^\dagger_{\mathbf{k}} p_{\mathbf{k}} + \frac{\omega^2_{\mathbf{k}}}{8\pi c^2} q^\dagger_{\mathbf{k}} q_{\mathbf{k}} = \frac{\hbar\omega_{\mathbf{k}}}{2}\left(P^\dagger_{\mathbf{k}} P_{\mathbf{k}} + Q^\dagger_{\mathbf{k}} Q_{\mathbf{k}}\right) \tag{65}$$

Here because it is a quantum problem, we suppose that the terms from $\mathbf{k}$ and $-\mathbf{k}$ modes really are not the same. Thus there is a similar term for the negative wave vector:

$$H_{-\mathbf{k}\alpha} = 2\pi c^2 p^\dagger_{-\mathbf{k}} p_{-\mathbf{k}} + \frac{\omega^2_{\mathbf{k}}}{8\pi c^2} q^\dagger_{-\mathbf{k}} q_{-\mathbf{k}} = \frac{\hbar\omega_{\mathbf{k}}}{2}\left(P^\dagger_{-\mathbf{k}} P_{-\mathbf{k}} + Q^\dagger_{-\mathbf{k}} Q_{-\mathbf{k}}\right) \tag{66}$$

The right hand sides are the same as the energies for SHO's in the normalized coordinates and momenta. However, we have relations like $q^\dagger_{-\mathbf{k}} = q_{\mathbf{k}}$, and $q_{-\mathbf{k}} = q^\dagger_{\mathbf{k}}$, and we suppose they should apply to the new rescaled coordinates and momenta. So this latter relation also takes the form

$$H_{-\mathbf{k}\alpha} = 2\pi c^2 p_{\mathbf{k}} p^\dagger_{\mathbf{k}} + \frac{\omega^2_{\mathbf{k}}}{8\pi c^2} q_{\mathbf{k}} q^\dagger_{\mathbf{k}} = \frac{\hbar\omega_{\mathbf{k}}}{2}\left(P_{\mathbf{k}} P^\dagger_{\mathbf{k}} + Q_{\mathbf{k}} Q^\dagger_{\mathbf{k}}\right) \tag{67}$$

In the quantum problem, the order in which conjugate operators act is important and should not be modified. So $H_{+\mathbf{k}\alpha}$ and $H_{-\mathbf{k}\alpha}$ are not the same. To match the sides, try the identifications

$$P_{\mathbf{k}} = \sqrt{\frac{4\pi c^2}{\hbar\omega_{\mathbf{k}}}} p_{\mathbf{k}}, \qquad Q_{\mathbf{k}} = \sqrt{\frac{\omega_{\mathbf{k}}}{4\pi c^2\hbar}} q_{\mathbf{k}} \tag{68}$$

The basic commutator that results between them is now unit normalized,

$$[Q_{\mathbf{k}}, P^\dagger_{\mathbf{k}}] = \sqrt{\frac{\omega_{\mathbf{k}}}{4\pi c^2\hbar}}\sqrt{\frac{4\pi c^2}{\hbar\omega_{\mathbf{k}}}}[q_{\mathbf{k}}, p^\dagger_{\mathbf{k}}] = \frac{1}{\hbar} i\hbar = i \tag{69}$$

It is obvious one can also show

$$[Q^\dagger_{\mathbf{k}}, P_{\mathbf{k}}] = i \tag{70}$$

Now we can re-express the energy in the sense of operators like what was done for the SHO, although it is more complicated here because of the two directions for the wavevectors. Note the following algebra that results if we try that, for complex operators:

$$\begin{aligned} F_1 &= \frac{1}{2}\left[(Q_{\mathbf{k}}+iP_{\mathbf{k}})(Q^\dagger_{\mathbf{k}}-iP^\dagger_{\mathbf{k}})+(Q^\dagger_{\mathbf{k}}-iP^\dagger_{\mathbf{k}})(Q_{\mathbf{k}}+iP_{\mathbf{k}})\right] \\ &= Q^\dagger_{\mathbf{k}}Q_{\mathbf{k}}+P^\dagger_{\mathbf{k}}P_{\mathbf{k}}+\frac{i}{2}\left[P_{\mathbf{k}}Q^\dagger_{\mathbf{k}}+Q^\dagger_{\mathbf{k}}P_{\mathbf{k}}-P^\dagger_{\mathbf{k}}Q_{\mathbf{k}}-Q_{\mathbf{k}}P^\dagger_{\mathbf{k}}\right] \end{aligned} \tag{71}$$

That has extra terms that we do not want. To get rid of them, consider also the contribution from the opposite wave vector. We use the same form, but with $-\mathbf{k}$, and employing $Q_{-\mathbf{k}}=Q^\dagger_{\mathbf{k}}$, $P_{-\mathbf{k}}=P^\dagger_{\mathbf{k}}$.

$$\begin{aligned} F_2 &= \frac{1}{2}\left[(Q_{-\mathbf{k}}+iP_{-\mathbf{k}})(Q^\dagger_{-\mathbf{k}}-iP^\dagger_{-\mathbf{k}})+(Q^\dagger_{-\mathbf{k}}-iP^\dagger_{-\mathbf{k}})(Q_{-\mathbf{k}}+iP_{-\mathbf{k}})\right] \\ &= \frac{1}{2}\left[(Q^\dagger_{\mathbf{k}}+iP^\dagger_{\mathbf{k}})(Q_{\mathbf{k}}-iP_{\mathbf{k}})+(Q_{\mathbf{k}}-iP_{\mathbf{k}})(Q^\dagger_{\mathbf{k}}+iP^\dagger_{\mathbf{k}})\right] \\ &= Q^*_{\mathbf{k}}Q_{\mathbf{k}}+P^*_{\mathbf{k}}P_{\mathbf{k}}-\frac{i}{2}\left[P_{\mathbf{k}}Q^\dagger_{\mathbf{k}}+Q^\dagger_{\mathbf{k}}P_{\mathbf{k}}-P^\dagger_{\mathbf{k}}Q_{\mathbf{k}}-Q_{\mathbf{k}}P^\dagger_{\mathbf{k}}\right] \end{aligned} \tag{72}$$

So the combination of the two expressions eliminates the imaginary part, leaving only the part we want in the Hamiltonian. Therefore, algebraically speaking we can write:

$$H_{+\mathbf{k}\alpha}=\frac{\hbar\omega_{\mathbf{k}}}{2}\frac{1}{2}(F_1+F_2) \tag{73}$$

Based on these expressions, introduce creation and annihilation operators, for both the positive and negative wave vectors:

$$a_{\mathbf{k}}=\frac{1}{\sqrt{2}}(Q_{\mathbf{k}}+iP_{\mathbf{k}}),\qquad a^\dagger_{\mathbf{k}}=\frac{1}{\sqrt{2}}(Q^\dagger_{\mathbf{k}}-iP^\dagger_{\mathbf{k}}). \tag{74}$$

$$a_{-\mathbf{k}}=\frac{1}{\sqrt{2}}(Q^\dagger_{\mathbf{k}}+iP^\dagger_{\mathbf{k}}),\qquad a^\dagger_{-\mathbf{k}}=\frac{1}{\sqrt{2}}(Q_{\mathbf{k}}-iP_{\mathbf{k}}). \tag{75}$$

By their definitions, they must have unit real commutators, e.g.,

$$[a_{\mathbf{k}},a^\dagger_{\mathbf{k}}]=\frac{1}{\sqrt{2}^2}[Q_{\mathbf{k}}+iP_{\mathbf{k}},Q^\dagger_{\mathbf{k}}-iP^\dagger_{\mathbf{k}}]=\frac{1}{2}\left\{-i[Q_{\mathbf{k}},P^\dagger_{\mathbf{k}}]+i[P_{\mathbf{k}},Q^\dagger_{\mathbf{k}}]\right\}=1 \tag{76}$$

On the other hand, a commutator between different modes (or with different polarizations at one wave vector) gives zero. The individual term in the Hamiltonian sum is

$$H_{+\mathbf{k}\alpha}=\frac{\hbar\omega_{\mathbf{k}}}{2}\frac{1}{2}\left[a_{\mathbf{k}}a^\dagger_{\mathbf{k}}+a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+a_{-\mathbf{k}}a^\dagger_{-\mathbf{k}}+a^\dagger_{-\mathbf{k}}a_{-\mathbf{k}}\right] \tag{77}$$

So the total field Hamiltonian is the sum

$$H=\sum_{\mathbf{k}}\frac{\hbar\omega_{\mathbf{k}}}{2}\left[a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+1/2+a^\dagger_{-\mathbf{k}}a_{-\mathbf{k}}+1/2\right] \tag{78}$$

The sum is over all wave vectors, and the positive and negative terms give the same total, so

$$H=\sum_{\mathbf{k}\alpha}\hbar\omega_{\mathbf{k}}\left(a^\dagger_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}+\frac{1}{2}\right)=\sum_{\mathbf{k}\alpha}\left(n_{\mathbf{k}\alpha}+\frac{1}{2}\right) \tag{79}$$

The number operator is implicitly defined here:

$$n_{\mathbf{k}\alpha}=a^\dagger_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha} \tag{80}$$

Then each mode specified by a wave vector and a polarization contributes $\hbar\omega(a^\dagger_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}+1/2)$ to the Hamiltonian. Every mode is equivalent, mathematically, to a simple harmonic oscillator. What

could be more simple? Really, it is hard to believe, when you think about it. The modes are completely independent, at this level, they do not interfere. There is just a linear superposition of their EM fields. To get those fields, summarize a few more relationships.

The fields associated with the creation and annihilation operators are found via solving their definitions,

$$Q_{\mathbf{k}} = \frac{1}{\sqrt{2}}(a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}}), \qquad P_{\mathbf{k}} = \frac{1}{i\sqrt{2}}(a_{\mathbf{k}} - a^\dagger_{-\mathbf{k}}), \tag{81}$$

Then with

$$\mathbf{A}_{\mathbf{k}\alpha} = A_{\mathbf{k}\alpha}\hat{\epsilon}_{\mathbf{k}\alpha}, \qquad A_{\mathbf{k}\alpha} = q_{\mathbf{k}\alpha} = \sqrt{\frac{4\pi c^2\hbar}{\omega_{\mathbf{k}}}}Q_{\mathbf{k}\alpha}, \tag{82}$$

applied into (19), the quantized fields are determined,

$$\mathbf{A}(\mathbf{r},t) = \frac{1}{2\sqrt{V}}\sum_{\mathbf{k}}\hat{\epsilon}_{\mathbf{k}\alpha}\left\{\sqrt{\frac{4\pi c^2\hbar}{\omega_{\mathbf{k}}}}\,\frac{(a_{\mathbf{k}\alpha} + a^\dagger_{-\mathbf{k}\alpha})}{\sqrt{2}}e^{i\mathbf{k}\cdot\mathbf{r}} + \sqrt{\frac{4\pi c^2\hbar}{\omega_{\mathbf{k}}}}\,\frac{(a_{-\mathbf{k}\alpha} + a^\dagger_{\mathbf{k}\alpha})}{\sqrt{2}}e^{-i\mathbf{k}\cdot\mathbf{r}}\right\} \tag{83}$$

Swapping some terms between the positive and negative wave vector sums, this is the same as

$$\mathbf{A}(\mathbf{r},t) = \sqrt{\frac{2\pi c^2\hbar}{V}}\sum_{\mathbf{k}}\frac{\hat{\epsilon}_{\mathbf{k}\alpha}}{\sqrt{\omega_{\mathbf{k}}}}\left[a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} + a^\dagger_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{84}$$

Then the vector potential determines both the electric and magnetic fields by (20) and (21), which give

$$\mathbf{E}(\mathbf{r},t) = i\sqrt{\frac{2\pi\hbar}{V}}\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}\hat{\epsilon}_{\mathbf{k}\alpha}}{\sqrt{\omega_{\mathbf{k}}}}\left[a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{85}$$

$$\mathbf{B}(\mathbf{r},t) = i\sqrt{\frac{2\pi\hbar}{V}}\sum_{\mathbf{k}}\frac{c\mathbf{k}\times\hat{\epsilon}_{\mathbf{k}\alpha}}{\sqrt{\omega_{\mathbf{k}}}}\left[a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{86}$$

Indeed, after all this work, the fields have a certain simplicity. Their amplitude depends on Planck's constant. Thus there must be quantum fluctuations determined by it.

The above do not show the explicit time dependence. However, that is implicit in the creation/annihilation operators. Based on the Hamiltonian, their equations of motion are simple:

$$i\hbar\dot{a}_{\mathbf{k}\alpha} = [a_{\mathbf{k}\alpha}, H] = \hbar\omega_{\mathbf{k}}[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}] = \hbar\omega_{\mathbf{k}}[a_{\mathbf{k}\alpha}, a^\dagger_{\mathbf{k}\alpha}]a_{\mathbf{k}\alpha} = +\hbar\omega_{\mathbf{k}}a_{\mathbf{k}\alpha} \tag{87}$$

$$i\hbar\dot{a}^\dagger_{\mathbf{k}\alpha} = [a^\dagger_{\mathbf{k}\alpha}, H] = \hbar\omega_{\mathbf{k}}[a^\dagger_{\mathbf{k}\alpha}, a^\dagger_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}] = \hbar\omega_{\mathbf{k}}a^\dagger_{\mathbf{k}\alpha}[a^\dagger_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}] = -\hbar\omega_{\mathbf{k}}a^\dagger_{\mathbf{k}\alpha} \tag{88}$$

And then they oscillate at opposite frequencies:

$$\dot{a}_{\mathbf{k}\alpha} = -i\omega_{\mathbf{k}}a_{\mathbf{k}\alpha} \Longrightarrow a_{\mathbf{k}\alpha}(t) = a_{\mathbf{k}\alpha}(0)e^{-i\omega_{\mathbf{k}}t} \tag{89}$$

$$\dot{a}^\dagger_{\mathbf{k}\alpha} = +i\omega_{\mathbf{k}}a^\dagger_{\mathbf{k}\alpha} \Longrightarrow a^\dagger_{\mathbf{k}\alpha}(t) = a^\dagger_{\mathbf{k}\alpha}(0)e^{+i\omega_{\mathbf{k}}t} \tag{90}$$

1.5 Quantized field properties: momentum, angular momentum

The fields not only carry energy, but it is directed, so they carry linear momentum and even angular momentum. The linear momentum is

$$\begin{aligned}\mathbf{G} = \int d^3\mathbf{r}\,\frac{\mathbf{E}\times\mathbf{B}}{4\pi c} \quad &= \quad \frac{i^2}{4\pi c}\frac{hc}{V}\sum_{\mathbf{k}\alpha}\sum_{\mathbf{k}'\alpha'}[\hat{\epsilon}_{\mathbf{k}\alpha}\times(\mathbf{k}'\times\hat{\epsilon}_{\mathbf{k}'\alpha'})]\times \\ &\int d^3\mathbf{r}\,(a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}})(a_{\mathbf{k}'\alpha'}e^{i\mathbf{k}'\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}'\alpha'}e^{-i\mathbf{k}'\cdot\mathbf{r}})\end{aligned} \tag{91}$$

The orthognality relation only gives nonzero terms where $\mathbf{k}' = \mathbf{k}$ and $\mathbf{k}' = -\mathbf{k}$, and there results

$$\mathbf{G} = \frac{hc}{4\pi} \sum_{\mathbf{k}\alpha} \sum_{\mathbf{k}'\alpha'} [\hat{\epsilon}_{\mathbf{k}\alpha} \times (\mathbf{k}' \times \hat{\epsilon}_{\mathbf{k}'\alpha'})] \left\{ (a_{\mathbf{k}\alpha} a^\dagger_{\mathbf{k}'\alpha'} + a^\dagger_{\mathbf{k}\alpha} a_{\mathbf{k}'\alpha'}) \delta_{\mathbf{k},\mathbf{k}'} - (a_{\mathbf{k}\alpha} a_{\mathbf{k}'\alpha'} + a^\dagger_{\mathbf{k}\alpha} a^\dagger_{\mathbf{k}'\alpha'}) \delta_{\mathbf{k},-\mathbf{k}'} \right\} \quad (92)$$

The orthogonality of the polarization vectors with each other and with $\mathbf{k}$ forces that vector cross product to be just $\mathbf{k}\delta_{\alpha,\alpha'}$. Only the direct terms give a nonzero result:

$$\mathbf{G} = \frac{hc}{4\pi} \sum_{\mathbf{k}\alpha} \mathbf{k} (a_{\mathbf{k}\alpha} a^\dagger_{\mathbf{k}\alpha} + a^\dagger_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha}) = \sum_{\mathbf{k}\alpha} \hbar c \mathbf{k} \; a^\dagger_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha} \quad (93)$$

There is no zero point term, because of the cancellation between a term at $+\mathbf{k}$ and one at $-\mathbf{k}$. Then each mode carries a linear momentum of $\hbar c\mathbf{k}$.

Consider the angular momentum. The contribution from the fields is

$$\mathbf{J} = \frac{1}{4\pi c} \int d^3\mathbf{r} \; [\mathbf{r} \times (\mathbf{E} \times \mathbf{B})] \quad (94)$$

But there is the identity,

$$[\mathbf{r} \times (\mathbf{E} \times \mathbf{B})] = \mathbf{E}(\mathbf{r} \cdot \mathbf{B}) - (\mathbf{r} \cdot \mathbf{E})\mathbf{B}. \quad (95)$$

Furthermore, for any mode, the wave vector is perpendicular to both $\mathbf{E}$ and $\mathbf{B}$. So this definition of angular momentum seems to give zero for the total component along the direction of propagation. Even if it more properly symmetrized for the QM problem, it still gives zero.

That shows that the concept of angular momentum in an EM field is tricky. Possibly, assuming a plane wave is too restrictive, and instead one should not make any particular assumption on the nature of the fields, to start with. One can do a more careful analysis, that shows the angular momentum is composed from an orbital part and a spin part.

Consider the following vector algebra for the ith component of the argument in the angular momentum integral (essentially, the angular momentum density). Here the Levi-Civita symbol is used for the cross products, and the magnetic field is expressed via the vector potential. Repeated indeces are summer over.

$$\begin{aligned} [\mathbf{r} \times (\mathbf{E} \times \mathbf{B})]_i &= \varepsilon_{ijk}\, x_j (\mathbf{E} \times \mathbf{B})_k = \varepsilon_{ijk}\, x_j \; \varepsilon_{klm}\, E_l B_m \\ &= \varepsilon_{ijk}\, x_j \; \varepsilon_{klm}\, E_l \; (\varepsilon_{mnp} \partial_n A_p) \\ &= \varepsilon_{ijk}\, x_j \; E_l (\delta_{kn}\delta_{lp} - \delta_{kp}\delta_{ln}) \partial_n A_p \\ &= \varepsilon_{ijk}\, x_j \; [E_l \partial_k A_l - E_l \partial_l A_k] \end{aligned} \quad (96)$$

Now when this is integrated over all space, the last term can be integrated by parts, dropping any vanishing surface terms at infinity. Further, far from any sources, the electric field is divergenceless, so $\vec{\nabla} \cdot \mathbf{E} = \partial_l E_l = 0$. So now the expression becomes

$$\begin{aligned} [\mathbf{r} \times (\mathbf{E} \times \mathbf{B})]_i &= \varepsilon_{ijk} \, [x_j E_l \partial_k A_l + \partial_l (x_j E_l) A_k] = \varepsilon_{ijk} \, [x_j E_l \partial_k A_l + \delta_{lj} E_l A_k] \\ &= \varepsilon_{ijk} \, [x_j E_l \partial_k A_l + E_j A_k] = E_l (\varepsilon_{ijk}\, x_j \partial_k) \, A_l + \varepsilon_{ijk}\, E_j A_k \end{aligned} \quad (97)$$

This is an interesting expression. The first term contains effectively the orbital angular momentum operator acting between $\mathbf{E}$ and $\mathbf{A}$. The second term is their cross product. Then the total angular momentum integrated over space is

$$\mathbf{J} = \frac{1}{4\pi c} \int d^3\mathbf{r} \; \{E_l (\mathbf{r} \times \nabla) A_l + \mathbf{E} \times \mathbf{A}\} \quad (98)$$

Both terms can be written as operators acting between the fields, adding $\hbar$ in appropriate places:

$$[\mathbf{r} \times (\mathbf{E} \times \mathbf{B})]_i = \frac{i}{\hbar} \{E_l (-i\hbar\, \varepsilon_{ijk}\, x_j \partial_k) A_l + E_j (-i\hbar\, \varepsilon_{ijk}\,) A_k\} \quad (99)$$

The first term in (99) contains the orbital angular momentum operator, $\mathbf{L}_i = (\mathbf{r}\times\mathbf{p})_i$, acting on identical components of $\mathbf{E}$ and $\mathbf{A}$; it is a diagonal operator. The second contains what is a spin-1 operator, for which one can write its $i^{\rm th}$ component,

$$(S_i)_{jk} = -i\hbar\,\varepsilon_{ijk}, \qquad (\mathbf{S})_{jk} = (S_i\hat{x}_i)_{jk} = -i\hbar\,\hat{x}_i\varepsilon_{ijk}. \tag{100}$$

Then the total angular momentum is expressed as a sum of these two parts, each being matrix elements of an operator,

$$\mathbf{J} = \frac{i}{4\pi\hbar c}\int d^3\mathbf{r}\;E_j\left[(\mathbf{r}\times\mathbf{p})\delta_{jk} + (\mathbf{S})_{jk}\right]A_k \tag{101}$$

Well, really $(S_i)_{jk}$ comes from the cross product operator, however, it can be seen to be a quantum spin operator, that couples different components of $\mathbf{E}$ and $\mathbf{A}$. This operator is defined here by its matrices, one for each component i, where j and k are the column and row

$$\begin{array}{c}(S_i)_{jk}\\(i=x,y,z)\end{array} = -i\hbar\varepsilon_{ijk} = -i\hbar\begin{pmatrix}0&0&0\\0&0&1\\0&-1&0\end{pmatrix}, -i\hbar\begin{pmatrix}0&0&-1\\0&0&0\\1&0&0\end{pmatrix}, -i\hbar\begin{pmatrix}0&1&0\\-1&0&0\\0&0&0\end{pmatrix}. \tag{102}$$

Check some properties to be convinced that this is really a spin-1 operator. Consider a commutator between two of these, using the properties of the Levi-Civita symbol. Start from the matrix multiplications, giving the $ln^{\rm th}$ element of the matrix products:

$$[(S_i)(S_j)]_{ln} = (S_i)_{lm}(S_j)_{mn} = (-i\hbar)^2\varepsilon_{ilm}\,\varepsilon_{jmn} = (-i\hbar)^2(\delta_{in}\delta_{lj} - \delta_{ij}\delta_{ln}) \tag{103}$$

$$[(S_j)(S_i)]_{ln} = (S_j)_{lm}(S_i)_{mn} = (-i\hbar)^2\varepsilon_{jlm}\,\varepsilon_{imn} = (-i\hbar)^2(\delta_{jn}\delta_{li} - \delta_{ji}\delta_{ln}) \tag{104}$$

The difference cancels the last terms,

$$[(S_i)(S_j) - (S_j)(S_i)]_{ln} = (-i\hbar)^2(\delta_{in}\delta_{lj} - \delta_{jn}\delta_{li}) \tag{105}$$

Then the difference of deltas can be put back into a product of ε's.

$$[(S_i)(S_j) - (S_j)(S_i)]_{ln} = (-i\hbar)^2(-\varepsilon_{ijk})\varepsilon_{lnk} = i\hbar\varepsilon_{ijk}[-i\hbar\varepsilon_{kln}] = i\hbar\varepsilon_{ijk}(S_k)_{ln}. \tag{106}$$

Therefore these matrices do have the commutation relations for an angular momentum,

$$[(S_i),(S_j)] = i\hbar\,\varepsilon_{ijk}\,(S_k). \tag{107}$$

Also, look at the matrix of $\vec{S}^2$, within the space that the operators act:

$$(\vec{S}^2)_{ln} = (S_i)_{lm}(S_i)_{mn} = (-i\hbar)^2\varepsilon_{ilm}\varepsilon_{imn} = (-i\hbar)^2(\delta_{lm}\delta_{mn} - \delta_{ln}\delta_{mm}) \tag{108}$$

The expression is summed over $m = x, y, z$, both the terms are diagonal. But $\delta_{lm}\delta_{mn} = \delta_{ln}$, while $\delta_{mm} = 3$. Then this square is the diagonal matrix:

$$(\vec{S}^2)_{ln} = (-i\hbar)^2(\delta_{ln} - 3\delta_{ln}) = 2\hbar^2\delta_{ln}. \tag{109}$$

This clearly has $s(s+1) = 2$ with $s = 1$, so indeed it corresponds to spin-1.

It may seem curious, that none of the matrices are diagonal. But this just means that the Cartesian axes, to which these correspond, are not the good quantization axes. For example, find the eigenvectors of the operator (S_x). The eigenvalue problem is

$$(S_x - \lambda I)(u) = \begin{pmatrix}-\lambda&0&0\\0&-\lambda&-i\hbar\\0&i\hbar&-\lambda\end{pmatrix}\begin{pmatrix}u_x\\u_y\\u_z\end{pmatrix} = 0. \tag{110}$$

The eigenvalues are obviously $\lambda = 0, \pm\hbar$. The $s_x = 0$ eigenvector is trivial, $u = (1,0,0)$, and seems to have little physical importance. The $s_x = +\hbar$ eigenvector is $u = \frac{1}{\sqrt{2}}(0,1,i)$ and the

$s_x = -\hbar$ eigenvector is $u = \frac{1}{\sqrt{2}}(0, 1, -i)$. If the vector potential were expressed in these as a basis, the spin angular momentum components along x are specified. But this basis is not the pure Cartesian components. It requires linear combinations of Cartesian components out of phase by $\pm 90°$. These combinations are states of circular polarization, which are the "good" states of spin angular momentum. Thus, none of these three matrices is diagonal when expressed in Cartesian components. More on the spin angular momentum and EM-wave polarization is discussed in the next section.

Note, if one had seeked the eigenvectors of the matrix (S_z), one finds they are $u = (0, 0, 1)$ for $s_z = 0$, and $u = (1, i, 0)$ for $s_z = +\hbar$, and $u = (1, -i, 0)$ for $s_z = -\hbar$. These last two correspond to states where the $\mathbf{A}$ and $\mathbf{E}$ fields are rotating around the z-axis. It is typical to consider waves propagating along z, hence, we see these vectors appear again when polarization is discussed for this wave vector direction.

Thus the second part of the angular momentum involves just the cross product of $\mathbf{E}$ and $\mathbf{A}$, which is considered the intrinsic *spin angular momentum* in the EM fields. It can seen to be the same as the canonical angular momentum in the fields, although it is hard to say in general why this is true. If one uses a definition like (coordinate $\times$ conjugate momentum), integrated over space, where the coordinate is the vector potential, and its conjugate momentum is $-\mathbf{E}/4\pi c$, one gets

$$\mathbf{S} = \int d^3\mathbf{r}\ \mathbf{A} \times \frac{-\mathbf{E}}{4\pi c} = \frac{-1}{4\pi c} \int d^3\mathbf{r}\ (\mathbf{A} \times \mathbf{E}) \tag{111}$$

Except for the ordering, it is the same as $\mathbf{S}$ obtained above. Assume the ordering doesn't matter (both are fields depending on position), and continue to evaluate it,

$$\mathbf{S} = \frac{-1}{4\pi c} \frac{ihc}{V} \sum_{\mathbf{k}\alpha} \sum_{\mathbf{k}'\alpha'} \hat{\epsilon}_{\mathbf{k}\alpha} \times \hat{\epsilon}_{\mathbf{k}'\alpha'} \int d^3\mathbf{r}\ \left[a_{\mathbf{k}\alpha} e^{i\mathbf{k}\cdot\mathbf{r}} + a^\dagger_{\mathbf{k}\alpha} e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \left[a_{\mathbf{k}'\alpha'} e^{i\mathbf{k}'\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}'\alpha'} e^{-i\mathbf{k}'\cdot\mathbf{r}}\right] \tag{112}$$

The integrations are the usual orthogonality relations, which give terms where $\mathbf{k}' = \mathbf{k}$ and terms where $\mathbf{k}' = -\mathbf{k}$. Only the first set gives nonzero results, due to the cross products of the polarization vectors (Take them oppositely directed for the $-\mathbf{k}$ mode compared to the $\mathbf{k}$ mode. Further, we look for a quantity whose expectation value is nonzero.) So there remains only the terms

$$\mathbf{S} = \frac{ih}{4\pi} \sum_{\mathbf{k}\alpha\alpha'} \hat{\epsilon}_{\mathbf{k}\alpha} \times \hat{\epsilon}_{\mathbf{k}\alpha'} (a_{\mathbf{k}\alpha} a^\dagger_{\mathbf{k}\alpha'} - a^\dagger_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha'}) \tag{113}$$

Here the two polarizations must be different to give a nonzero result. We suppose they are oriented in such a way that

$$\hat{\epsilon}_{\mathbf{k}1} \times \hat{\epsilon}_{\mathbf{k}2} = \hat{k} \tag{114}$$

so that this cross product is along the propagation direction. Then there are two equal terms and the net is

$$\mathbf{S} = \sum_{\mathbf{k}} i\hbar\hat{k}\ (a_{\mathbf{k}1} a^\dagger_{\mathbf{k}2} - a^\dagger_{\mathbf{k}1} a_{\mathbf{k}2}) \tag{115}$$

As shown with the eigenvalues of the S matrices, the basic unit of spin angular momentum is $\hbar$, and it has a component only along (or opposite to) the propagation direction.

1.6 Orbital angular momentum

Mostly in atomic processes, the spin angular momentum is absorbed or emitted when photons are absorbed or emitted by atoms. Not much is usually mentioned about the orbital angular momentum in the EM fields. Consider here what $\mathbf{L}$ is for the quantized EM field, using the expression,

$$\mathbf{L} = \frac{1}{4\pi c} \int d^3\mathbf{r}\ E_l (\mathbf{r} \times \nabla) A_l. \tag{116}$$

If the ∇ operation is applied to the fields in (84), it pulls out $i\mathbf{k}$ for each mode. One then has

$$(\mathbf{r}\times\nabla)A_l = \sqrt{\frac{2\pi c^2\hbar}{V}}\sum_{\mathbf{k}}\frac{\hat{x}_l\cdot\hat{\epsilon}_{\mathbf{k}\alpha}}{\sqrt{\omega_{\mathbf{k}}}}\mathbf{r}\times(i\mathbf{k})\left[a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{117}$$

Now combine with the same component of the electric field,

$$\begin{aligned} E_l(\mathbf{r}\times\nabla)A_l &= i\sqrt{\frac{2\pi\hbar}{V}}\sum_{\mathbf{k}'\alpha'}\frac{\omega_{\mathbf{k}'}\hat{x}_l\cdot\hat{\epsilon}_{\mathbf{k}'\alpha'}}{\sqrt{\omega_{\mathbf{k}'}}}\left[a_{\mathbf{k}'\alpha'}e^{i\mathbf{k}'\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}'\alpha'}e^{-i\mathbf{k}'\cdot\mathbf{r}}\right] \\ &\times \sqrt{\frac{2\pi c^2\hbar}{V}}\sum_{\mathbf{k}\alpha}\frac{\hat{x}_l\cdot\hat{\epsilon}_{\mathbf{k}\alpha}}{\sqrt{\omega_{\mathbf{k}}}}\mathbf{r}\times(i\mathbf{k})\left[a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \end{aligned} \tag{118}$$

The orbital angular momentum then is

$$\mathbf{L} = \frac{ih}{4\pi V}\sum_{\mathbf{k},\mathbf{k}',\alpha\alpha'}\sqrt{\frac{\omega_{\mathbf{k}'}}{\omega_{\mathbf{k}}}}\hat{\epsilon}_{\mathbf{k}'\alpha'}\cdot\hat{\epsilon}_{\mathbf{k}\alpha}\int d^3\mathbf{r}\ \mathbf{r}\left[a_{\mathbf{k}'\alpha'}e^{i\mathbf{k}'\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}'\alpha'}e^{-i\mathbf{k}'\cdot\mathbf{r}}\right]\left[a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} - a^\dagger_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}}\right]\times(i\mathbf{k}) \tag{119}$$

The basic integral to evaluate here is not exactly a normalization integral:

$$I_x = \int d^3\mathbf{r}\ xe^{i\mathbf{k}'\cdot\mathbf{r}}e^{i\mathbf{k}\cdot\mathbf{r}} = -i\frac{\partial}{\partial k_x}\int d^3\mathbf{r}\ e^{i\mathbf{k}'\cdot\mathbf{r}}e^{i\mathbf{k}\cdot\mathbf{r}} = -i\frac{\partial}{\partial k_x}V\delta_{\mathbf{k},\mathbf{k}'} \tag{120}$$

It would seem to be zero, although singular in some sense. For now I'll consider that the orbital angular momentum should be zero.

One thing that can be said with more certainty is the component of $\mathbf{L}$ along the propagation direction, $\mathbf{k}$, for some mode in the sum. As $[\mathbf{r}\times(i\mathbf{k})]\cdot\mathbf{k} = 0$, for a particular mode, there is no orbital angular momentum component in the direction of propagation.

1.7 Polarization

It is better to express the spin angular momentum $\mathbf{S}$ in terms of circular polarization components. In the expressions for $\mathbf{E}$, the cartesian polarization vectors could be re-expressed in terms of rotating basis vectors. For example, consider a wave moving in the z direction, with $\hat{\epsilon}_1 = \hat{x}$ and $\hat{\epsilon}_2 = \hat{y}$. Then if you look at, for example,

$$(\hat{x} + i\hat{y})e^{-i\omega t} = (\hat{x}\cos\omega t + \hat{y}\sin\omega t) + i(-\hat{x}\sin\omega t + \hat{y}\cos\omega t) \tag{121}$$

At $t = 0$, the real part is along $\hat{x}$ and the imaginary part is along $\hat{y}$. At time progresses, both the real and imaginary parts rotate counterclockwise when viewed in the usual xy-plane. I am supposing this multiplying the positive wave, $a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$. Then both of these rotate in the positive helicity sense, where the angular momentum is in the same direction as the wave propagation. The following wave rotates in the opposite sense, clockwise or negative helicity:

$$(\hat{x} - i\hat{y})e^{-i\omega t} = (\hat{x}\cos\omega t - \hat{y}\sin\omega t) + i(-\hat{x}\sin\omega t - \hat{y}\cos\omega t) \tag{122}$$

These suggest inventing polarization basis vectors for these two helicities (the wave vector index is suppressed),

$$\hat{\epsilon}_L = \hat{\epsilon}_+ = \frac{1}{\sqrt{2}}(\hat{\epsilon}_1 + i\hat{\epsilon}_2), \qquad \hat{\epsilon}_R = \hat{\epsilon}_- = \frac{1}{\sqrt{2}}(\hat{\epsilon}_1 - i\hat{\epsilon}_2) \tag{123}$$

I use L and R for left and right in place of positive and negative. The inverse relations are

$$\hat{\epsilon}_1 = \frac{1}{\sqrt{2}}(\hat{\epsilon}_L + \hat{\epsilon}_R), \qquad \hat{\epsilon}_2 = \frac{1}{i\sqrt{2}}(\hat{\epsilon}_L - \hat{\epsilon}_R) \tag{124}$$

Then we see that in the expression for the electric field, there appears a combination $\sum_\alpha \hat{\epsilon}_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}$, or

$$\hat{\epsilon}_1 a_{\mathbf{k}1} + \hat{\epsilon}_2 a_{\mathbf{k}2} = \frac{1}{\sqrt{2}}(\hat{\epsilon}_L + \hat{\epsilon}_R)a_{\mathbf{k}1} + \frac{1}{i\sqrt{2}}(\hat{\epsilon}_L - \hat{\epsilon}_R)a_{\mathbf{k}2} = \frac{1}{\sqrt{2}}(a_{\mathbf{k}1} - ia_{\mathbf{k}2})\hat{\epsilon}_L + \frac{1}{\sqrt{2}}(a_{\mathbf{k}1} + ia_{\mathbf{k}2})\hat{\epsilon}_R \tag{125}$$

This shows the two new alternative (circularly polarized) annihilation operators,

$$a_{\mathbf{k}L} \equiv \frac{1}{\sqrt{2}}(a_{\mathbf{k}1} - ia_{\mathbf{k}2}), \qquad a_{\mathbf{k}R} \equiv \frac{1}{\sqrt{2}}(a_{\mathbf{k}1} + ia_{\mathbf{k}2}). \tag{126}$$

Their inverse relations are

$$a_{\mathbf{k}1} = \frac{1}{\sqrt{2}}(a_{\mathbf{k}L} + a_{\mathbf{k}R}), \qquad a_{\mathbf{k}2} = \frac{i}{\sqrt{2}}(a_{\mathbf{k}L} - a_{\mathbf{k}R}). \tag{127}$$

Then a sum can be over either linear or circular basis:

$$\sum_\alpha \hat{\epsilon}_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha} = \hat{\epsilon}_1 a_{\mathbf{k}1} + \hat{\epsilon}_2 a_{\mathbf{k}2} = \hat{\epsilon}_L a_{\mathbf{k}L} + \hat{\epsilon}_R a_{\mathbf{k}R} \tag{128}$$

Additionally there are the corresponding creation operators,

$$a^\dagger_{\mathbf{k}L} \equiv \frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}1} + ia^\dagger_{\mathbf{k}2}), \qquad a^\dagger_{\mathbf{k}R} \equiv \frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}1} - ia^\dagger_{\mathbf{k}2}). \tag{129}$$

Their inverse relations are

$$a^\dagger_{\mathbf{k}1} = \frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}L} + a^\dagger_{\mathbf{k}R}), \qquad a^\dagger_{\mathbf{k}2} = \frac{-i}{\sqrt{2}}(a^\dagger_{\mathbf{k}L} - a^\dagger_{\mathbf{k}R}). \tag{130}$$

The expressions for the fields really don't depend on which basis is used. However, the ones stated earlier do need to be modified to be more general, since now the basis vectors can be complex. To be totally consistent for the creation terms, we need to satisfy the conjugate relation

$$\sum_\alpha \hat{\epsilon}^\dagger_{\mathbf{k}\alpha} a^\dagger_{\mathbf{k}\alpha} = \hat{\epsilon}^\dagger_1 a^\dagger_{\mathbf{k}1} + \hat{\epsilon}^\dagger_2 a^\dagger_{\mathbf{k}2} = \hat{\epsilon}^\dagger_L a^\dagger_{\mathbf{k}L} + \hat{\epsilon}^\dagger_R a^\dagger_{\mathbf{k}R} \tag{131}$$

It means that the correct expressions for the fields in the case of complex basis vectors must be

$$\mathbf{A}(\mathbf{r},t) = \sqrt{\frac{2\pi c^2\hbar}{V}} \sum_{\mathbf{k}} \frac{1}{\sqrt{\omega_{\mathbf{k}}}} \left[\hat{\epsilon}_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha} e^{i\mathbf{k}\cdot\mathbf{r}} + \hat{\epsilon}^\dagger_{\mathbf{k}\alpha} a^\dagger_{\mathbf{k}\alpha} e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{132}$$

$$\mathbf{E}(\mathbf{r},t) = i\sqrt{\frac{2\pi\hbar}{V}} \sum_{\mathbf{k}} \sqrt{\omega_{\mathbf{k}}} \left[\hat{\epsilon}_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha} e^{i\mathbf{k}\cdot\mathbf{r}} - \hat{\epsilon}^\dagger_{\mathbf{k}\alpha} a^\dagger_{\mathbf{k}\alpha} e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{133}$$

$$\mathbf{B}(\mathbf{r},t) = i\sqrt{\frac{2\pi\hbar}{V}} \sum_{\mathbf{k}} \frac{c\mathbf{k}\times}{\sqrt{\omega_{\mathbf{k}}}} \left[\hat{\epsilon}_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha} e^{i\mathbf{k}\cdot\mathbf{r}} - \hat{\epsilon}^\dagger_{\mathbf{k}\alpha} a^\dagger_{\mathbf{k}\alpha} e^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{134}$$

The combinations of operators with their conjugates shows that these totals are hermitian.

Now the expression for the spin angular mometum can be expressed using the circular components,

$$\mathbf{S} = \sum_{\mathbf{k}} i\hbar\hat{k} \left[\frac{1}{\sqrt{2}}(a_{\mathbf{k}L} + a_{\mathbf{k}R})\frac{-i}{\sqrt{2}}(a^\dagger_{\mathbf{k}L} - a^\dagger_{\mathbf{k}R}) - \frac{1}{\sqrt{2}}(a^\dagger_{\mathbf{k}L} + a^\dagger_{\mathbf{k}R})\frac{i}{\sqrt{2}}(a_{\mathbf{k}L} - a_{\mathbf{k}R})\right] \tag{135}$$

The different polarizations commute, and the only nonzero commutation relations for the circular polarization creation and annihilation operators are

$$[a_{\mathbf{k}L}, a^\dagger_{\mathbf{k}L}] = 1, \qquad [a_{\mathbf{k}R}, a^\dagger_{\mathbf{k}R}] = 1. \tag{136}$$

So all that survives after using the commutation relations is

$$\mathbf{S} = \sum_{\mathbf{k}} \hbar\hat{k} \left[a^\dagger_{\mathbf{k}L} a_{\mathbf{k}L} - a^\dagger_{\mathbf{k}R} a_{\mathbf{k}R}\right] \tag{137}$$

This apparently involves number operators for each circular polarization. The left states contribute $+\hbar\hat{k}$ and the right states contribute $-\hbar\hat{k}$ to the total angular momentum. So in a sense, one can consider that photons carry an intrinsic angular momentum of magnitude $\hbar$. Then they can be considered as particles with spin-1. The numbers operators in this expression count the number of photons in each helicity or circular polarization state.

The creation operators generate quanta of the EM field, in some sense. There are the linear polarization operators and the circular ones. We might think of the circular state as a linear combination of two linear states, and vice versa. Does a photon have an intrinsic angular momentum? Perhaps it is not a reasonable question. Depending on what is measured, you may only see either the linear components or only the circular components. The basis you would use is determined by how the experiment is performed, i.e., by what states your experiment projects out. However, some photon-atom interactions, for example, may be most sensitive to the circular components. Then that type of experiment would view the photons as having circular polarization and as being spin-1 particles.

2 Interactions of EM fields with matter

EM fields are always coupled to charged particles. Here coupling of the quantized EM field to nonrelativistic charges is considered. It is expected that this is a situation where a perturbation approach can be applied. It means, we think the eigenstates of some material problem are known, and we want to see the perturbations due to the application of light. Or, it could be we want to see the emission of light that is expected, either spontaneously due to fluctuations in the EM field, or stimulated by the EM field. This is a brief summary of how to go about these calculations.

The usual prescription to include interactions is to modify the four-momentum of the particle of charge q, according to the effects of the field it experiences,

$$\mathbf{p} \longrightarrow \mathbf{p} - \frac{q}{c}\mathbf{A}, \qquad E \longrightarrow E - qA_0 \tag{138}$$

where $\mathbf{A}$ is the vector potential and A_0 is the scalar potential ϕ. The energy operator is the usual $E = i\hbar\frac{\partial}{\partial t}$ and the momentum operator is the usual $\mathbf{p} = -i\hbar\nabla$. The original problem in the absence of the fields is a Schrödinger problem $H\Psi = E\Psi$,

$$\left[\frac{\mathbf{p^2}}{2m} + V(\mathbf{r})\right]\Psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) \tag{139}$$

When the EM fields are now turned on, this changes to

$$\left[\frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 + V(\mathbf{r}) + qA_0\right]\Psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) \tag{140}$$

Then the effective Hamiltonian for the perturbed problem is just

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 + V(\mathbf{r}) + qA_0 \tag{141}$$

The simplest case is to consider a single particle or charge as it interacts with the field. In addition, there is supposed to be the Hamiltonian for the free EM fields themselves, as we quantized in the previous section. So the total effective Hamiltonian for particle in the field is

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) - \frac{q}{2mc}(\mathbf{A}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{A}) + \frac{q^2\mathbf{A^2}}{2mc^2} + qA_0 + H_{\text{photons}} \tag{142}$$

The first two terms are the free particle, the next three terms are the interaction with the EM fields, and the last term is the free photon Hamiltonian, whose eigenstates are states with certain numbers of photons are given wavevectors and polarizations.

Although not necessary, we can continue to use the radiation gauge, where $\nabla\cdot\mathbf{A} = \mathbf{0}$ and $A_0 = 0$, as we used for the free photons. This implies $\mathbf{p}\cdot\mathbf{A} = \mathbf{A}\cdot\mathbf{p}$. Then there are only two interaction

terms, one that is linear in $\mathbf{A}$ and one that is quadratic in $\mathbf{A}$. The linear terms will involve individual photon creation and annihilation terms, corresponding to single-photon processes that can be analyzed in first order perturbation theory. The quadratic terms correspond to two-photon processes even in first order PT, and probably to get those correct would actually require second order PT. However, they should be smaller. Thus the leading perturbation is due to only the single-photon term,

$$H_1 = -\frac{q}{mc}\mathbf{A}\cdot\mathbf{p} + \frac{q^2\mathbf{A^2}}{2mc^2} \approx -\frac{q}{mc}\mathbf{A}\cdot\mathbf{p} \tag{143}$$

Note that the $\mathbf{A}$ operator is due to the EM field (creation/annihilation) while the $\mathbf{p}$ operator is associated with the charged particle momentum only. These would act on composite bra or kets involving both the EM field state and the particle state.

In a basic process where the final state has one less photon than the initial state, a photon was absorbed by the matter. On the other hand, if the final state has one more photon than the initial state, a photon was emitted by the matter.

In absorption, the absorbed photon could come from any direction $d\Omega$. In emission, the emitted photon can go out in any direction $d\Omega$. In either case, some density of states is involved in the calculation of the rate for the process, consistent with conservation of energy and other variables.

2.1 First order perturbations: single photon events

The amplitude for a transition between some initial and final states is given by a matrix element, which goes into Fermi's Golden Rule to get the transition rate:

$$w_{I\to F} = \frac{2\pi}{\hbar}\left|\langle\Psi_F|H_1|\Psi_I\rangle\right|^2\rho \tag{144}$$

where ρ is some density of states for the photon involved. The interaction can be written using the quantized EM field $\mathbf{A}$,

$$H_1 = \frac{-q}{mc}\sqrt{\frac{2\pi c^2\hbar}{V}}\sum_{\mathbf{k}}\frac{1}{\sqrt{\omega_{\mathbf{k}}}}\left[\hat{\epsilon}_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} + \hat{\epsilon}^\dagger_{\mathbf{k}\alpha}a^\dagger_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}}\right]\cdot\mathbf{p} \tag{145}$$

So we need matrix elements of this, between states with given numbers of photons, and initial and final states of the matter. Especially, the quantum process of light emission or absorption requires use of the basic matrix elements of the creation/annhilation operators.

The states are products of a state for the particle and a state for the fields. So we write in general,

$$|\Psi\rangle = |\psi\rangle|\ (n)\rangle \tag{146}$$

where ψ refers to the particle state, and (n) is a shorthand notation for the occupation numbers of all of the photon modes. In absorption or emission, we suppose that only one of the photon modes changes its occupation number, because we are dealing with single-photon processes. Then the general matrix element for the process is

$$\begin{aligned}\langle\Psi_F|H_1|\Psi_I\rangle = \frac{-q}{m}\sqrt{\frac{\hbar}{V}}\sum_{\mathbf{k}\alpha}\frac{1}{\sqrt{\omega_{\mathbf{k}}}} \qquad & \Big\{\langle(n)_f|a_{\mathbf{k}\alpha}e^{-i\omega_{\mathbf{k}}t}|(n)_i\rangle\langle\psi_f|e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\epsilon}_{\mathbf{k}\alpha}\cdot\mathbf{p}|\psi_i\rangle \\ & + \langle(n)_f|a^\dagger_{\mathbf{k}\alpha}e^{i\omega_{\mathbf{k}}t}|(n)_i\rangle\langle\psi_f|e^{-i\mathbf{k}\cdot\mathbf{r}}\hat{\epsilon}_{\mathbf{k}\alpha}\cdot\mathbf{p}|\psi_i\rangle\Big\}\end{aligned} \tag{147}$$

In first order time-dependent perturbation theory, if an effective potential that is acting is $V(t) = V_o e^{-i\omega t} + V_o^\dagger e^{+i\omega t}$, the transition amplitude according to the Born approximation is a matrix element,

$$\langle f|U(t,0)|i\rangle = \frac{-i}{\hbar}\int_0^t d\tau\ e^{i\omega_{fi}\tau}\langle f|V(\tau)|i\rangle, \qquad \omega_{fi} \equiv \frac{(E_f - E_i)}{\hbar} \tag{148}$$

That's the same form we have for this problem. The frequency here depends on the difference in energy of the initial and final states of the matter, which is being perturbed by the radiation.

Now when combined with the frequency of the radiation field (for one particular mode), the time integrations needed are simple, one for absorption or destruction of a photon, and one for emission or creation of a photon,

$$\int_0^t d\tau\ e^{i\omega_{fi}\tau} e^{-i\omega_{\mathbf{k}}\tau} = \frac{e^{i(\omega_{fi}-\omega_{\mathbf{k}})t}-1}{i(\omega_{fi}-\omega_{\mathbf{k}})}, \qquad \text{for absorption} \tag{149}$$

$$\int_0^t d\tau\ e^{i\omega_{fi}\tau} e^{+i\omega_{\mathbf{k}}\tau} = \frac{e^{i(\omega_{fi}+\omega_{\mathbf{k}})t}-1}{i(\omega_{fi}+\omega_{\mathbf{k}})}, \qquad \text{for emission} \tag{150}$$

These expressions tend to get large where the denominators go to zero. Since this occurs at different places, we can consider absorption and emission separately.

For Absorption: The squared matrix element is the probability to find the system in the desired final state after a time t has passed. When we let $t \to \infty$, and divide by the time, it gives the **transition rate**. This is one thing, for example, that can be calculated. In the problem of finding the dielectric function of a material, however, we will want to find some different quantities. Thus let's just summarize this briefly.

For simplicitly, supposed there is only one wavelength of light present in the radiation field, the one that is exactly tuned to be absorbed! The radiation matrix element that is needed is

$$\langle (n)_f | a_{\mathbf{k}\alpha} | (n)_i \rangle = \sqrt{n_{\mathbf{k}\alpha}} \tag{151}$$

This is an extreme approximation, because the light should really have some spectral distribution. This can be corrected later. Then the probability for absorbing this one mode is the squared matrix element (squared transition amplitude),

$$|\langle f|U|i\rangle|^2 = \frac{2\pi q^2 n_{\mathbf{k}\alpha}}{m^2 V \hbar\omega_{\mathbf{k}}} \left|\langle \psi_f | e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\epsilon}_{\mathbf{k}\alpha}\cdot\mathbf{p}|\psi_i\rangle\right|^2 \left[\frac{\sin\frac{(\omega_{fi}-\omega_{\mathbf{k}})}{2}t}{\frac{(\omega_{fi}-\omega_{\mathbf{k}})}{2}}\right]^2 \quad \text{(absorption)} \tag{152}$$

In the limit of large time, the last factor acts like a delta functon in its argument in the sine. So this result is particularly peaked at the resonance, $\omega_{\mathbf{k}} = \omega_{fi}$, which just displays the conservation of energy in the absorption process.

Now consider a certain spectrum of radiation, but all travelling in one direction (a beam). The sum over wave vector can be considered in this situation as an integral over only the magnitude of $\mathbf{k}$, or equivalently, over the frequency $\omega_{\mathbf{k}}$. The beam is characterized by the intensity of its light at different frequencies, i.e., its spectrum, which could be very narrow or very wide. Let a function $I_\alpha(\omega)$ describe the intensity of light per unit frequency interval. Then $I_\alpha(\omega)d\omega$ is the energy per time per area in the beam, for modes of frequency ω and polarization α. Also, intensity in waves is their energy density times their speed. For a collection of N monochromatic photons, the intensity could be written

$$I = \frac{N}{V}\hbar\omega c, \quad \Longrightarrow \quad N = V\frac{I}{\hbar\omega c} \tag{153}$$

Here we have a sum and not exactly monochromatic light. If we change a sum over modes into a continuous integral, we usually do the replacement,

$$\sum_{\mathbf{k}} \longrightarrow \frac{V}{(2\pi)^3}\int d^3\mathbf{k} \tag{154}$$

But that would apply to photons travelling in all possible directions. If we instead just sum up the photons, each of energy $\hbar\omega$ travelling at the speed c along the chosen beam direction, the number of photons (in volume V in the beam) will be described by

$$\sum_{\mathbf{k}} n_{\mathbf{k}\alpha} \longrightarrow V\int d\omega\ \frac{I_\alpha(\omega)}{\hbar\omega c} \tag{155}$$

The absorption transition rate involves the limit,

$$w = \lim_{t\to\infty} \frac{1}{t} \sum_{\mathbf{k}\alpha} |\langle f|U|i\rangle|^2 \tag{156}$$

For the matter in a beam of radiation, this leads to

$$w = \lim_{t\to\infty} \frac{1}{t} V \int d\omega \; \frac{I_\alpha(\omega)}{\hbar\omega c} \frac{2\pi q^2}{m^2 V\hbar\omega} \left|\langle\psi_f|e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\epsilon}_{\mathbf{k}\alpha}\cdot\mathbf{p}|\psi_i\rangle\right|^2 \left[\frac{\sin\frac{(\omega_{fi}-\omega)}{2}t}{\frac{(\omega_{fi}-\omega)}{2}}\right]^2 \tag{157}$$

When the limit is taken, the last function on the end produces a delta function enforcing $\omega = \omega_{fi}$. Using $x = \frac{(\omega_{fi}-\omega)}{2}t$, the weight is found to be

$$\frac{1}{t}\int_{-\infty}^{+\infty} d\omega \left[\frac{\sin\frac{(\omega_{fi}-\omega)}{2}t}{\frac{(\omega_{fi}-\omega)}{2}}\right]^2 = \int_{-\infty}^{+\infty} dx \; 2\left(\frac{\sin x}{x}\right)^2 = 2\pi \tag{158}$$

Therefore the transition rate for absorption of one polarization from the beam can be expressed

$$w = \frac{1}{c}\left(\frac{2\pi q}{m\hbar\omega_{fi}}\right)^2 I_\alpha(\omega_{fi}) \left|\langle\psi_f|e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\epsilon}_{\mathbf{k}\alpha}\cdot\mathbf{p}|\psi_i\rangle\right|^2 \qquad \text{(absorption)} \tag{159}$$

Emission: The radiation matrix element squared now is $n_{\mathbf{k}\alpha} + 1$. The first term corresponds to stimulated emission, caused by radiation already present, and the second is the spontaneious emission. The calculation of the stimulated rate follows the same algebra as for absorption. One will arrive at the rate in a beam to be

$$w = \frac{1}{c}\left(\frac{2\pi q}{m\hbar\omega_{if}}\right)^2 I_\alpha(\omega_{if}) \left|\langle\psi_f|e^{-i\mathbf{k}\cdot\mathbf{r}}\hat{\epsilon}_{\mathbf{k}\alpha}\cdot\mathbf{p}|\psi_i\rangle\right|^2 \qquad \text{(stimulated emission)} \tag{160}$$

So this is really now much different from the absorption expression. Physically, however, it is completely different, especialy, in that the rocess will produce a new photon that is coherent with the present photons. This leads to masers, lasers, etc. The produced photon is just a copy of one of the original ones, and is also travelling in the same direction.

For now I don't discuss spontaneous emission, although it is a very interesting subject!

3 Electric polarization and dielectrics

Here I want to consider the basic theory for induced electric dipoles in matter, and how that leads to the electric permitivity $\epsilon(\omega)$. In optical systems, it is clear that the response of a medium to the radiation fields, i.e., photons, induces electric dipoles, and those in turn could react back on the radiation. The theory is related to that just discussed for using time-dependent perturbation theory applied to absorption and emission of photons.

An optical medium has a dielectric response due primarily to its electrons of charge $q = -e$, and their dipole moments induced by applied fields. I will consider this as a quantum problem, because I will include the effects of both the electric and magnetic fields, especially, what happens when a DC magnetic field is applied (Faraday effect).

Start from the simplest problem, the Drude model, where the optical medium is composed just from a gas of free (noninteracting) electrons, moving between fixed nuclei. Classically the problem is quite simple: the electric field in the radiation field at frequency ω displaces the electrons from their original positions, at the frequency of the radiation. Then it is easy to find the induced dipoles and do the necessary electrodynamics to get $\epsilon(\omega)$. The only possible difficulty: the gas oscillates as a whole, leading to plasma oscillations. But we aren't really considering this kind of collective mode, only the averaged response of individual charges. An individual charge follows Newton's Law, in the net field surrounding it, $\mathbf{E} = \mathbf{E}_0 e^{-i\omega t}$,

$$m\ddot{\mathbf{r}} = q\mathbf{E}_0 e^{-i\omega t}, \quad \Longrightarrow \quad \mathbf{r}(t) = \frac{-q\mathbf{E}_0}{m\omega^2} e^{-i\omega t} = \frac{-q}{m\omega^2}\mathbf{E} \tag{161}$$

The charge oscillates at the same frequency as the radiation, and its displacements of amplitude $-q\mathbf{E}_0/m\omega^2$ about its original position are proportional to the strength of the radiation. The charge's induced electric dipole moment is $\mathbf{d} = q\mathbf{r}$. If there are N charges in a volume V, or a volume density of $n = N/V$, then the net dipole moment per unit volume is the electric polarization,

$$\mathbf{P} = n\mathbf{d} = nq\mathbf{r} = -\frac{nq^2}{m\omega^2}\mathbf{E} \tag{162}$$

The total electric displacement can then be found (CGS units) to get the dielectric function,

$$\mathbf{D} = \epsilon\mathbf{E} = \mathbf{E} + 4\pi\mathbf{P} = \left(1 - 4\pi\frac{nq^2}{m\omega^2}\right)\mathbf{E} \quad \Longrightarrow \epsilon(\omega) = 1 - 4\pi\frac{nq^2}{m\omega^2} \tag{163}$$

One can see the large oscillations and response will occur if $\epsilon \to 0$, which takes place at the plasma frequency,

$$\omega_p = \sqrt{\frac{4\pi nq^2}{m}} \tag{164}$$

Then it is usual to write the dielectric function for this simplest case as

$$\epsilon(\omega) = 1 - 4\pi\frac{nq^2}{m\omega^2} = 1 - \frac{\omega_p^2}{\omega^2} \tag{165}$$

Note that to convert the results to SI units, just recall that the charge must be re-scaled by the relation

$$q_{\text{CGS}}^2 \to \frac{q_{\text{SI}}^2}{4\pi\epsilon_0}; \qquad \omega_p = \sqrt{\frac{nq^2}{m\epsilon_0}} \quad \text{(SI units)} \tag{166}$$

where $\epsilon_0 = 8.854$ pF/m is the permitivity of vacuum. Furthermore, one can consider partially bound electrons with damped motion–it is a slight modification of the above and removes the infinite divergence at the plasma frequency.

What about the QM problem for the Drude model? The free electrons can be assumed to be in eigenstates of momentum, i.e, their unperturbed Hamiltonian only has kinetic energy:

$$H_{\text{e}} = \frac{\mathbf{p^2}}{2m} \tag{167}$$

Take the eigenstates as normalized plane waves:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}} \tag{168}$$

First I'll consider a zero temperature problem. Just consider the effects on an individual electron and its interaction with the quantized radiation fields in the Coulomb gauge. Take the interaction due to single-photon processes, as discussed in the previous section:

$$H_1 = -\frac{q}{mc}\mathbf{A}\cdot\mathbf{p} \tag{169}$$

The perturbation should cause the electron to make transitions between the plane wave states. Let's see what happens. We know the expression for the radiation vector potential, so

$$H_1 = \frac{-q}{m}\sqrt{\frac{h}{V}}\sum_{\mathbf{k}}\frac{1}{\sqrt{\omega_{\mathbf{k}}}}\left[\hat{\epsilon}_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}e^{i\mathbf{k}\cdot\mathbf{r}} + \hat{\epsilon}^{\dagger}_{\mathbf{k}\alpha}a^{\dagger}_{\mathbf{k}\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}}\right]\cdot\mathbf{p} \tag{170}$$

Now we don't necessarily need to know transition rates for this problem, we only want to know the expectation value of the electric dipole moment operator, $\mathbf{d} = q\mathbf{r}$. Unfortunately, we see right away, that for whatever state of the electron we might pick, this expectation will be zero, because of the photon operators. If the photon number does not change, the photon matrix elements will give zero.

Thus I suspect we need to look at this problem with second order perturbation theory. Further, we need to be cleaer about what is the actual state of the photons being considered. However, that could be fairly simple, say, a state with n identical photons (a very large number) at the frequency for which we need to know $\epsilon(\omega)$. Even for this state, first order PT will not give an induced dipole moment.

It's possible that states of the time-dependent Hamiltonian, $H_{\mathrm{e}} + H_1$ can be solved without a perturbation approach. Try that first.

Physics 195
Course Notes
Second Quantization
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1 Introduction

This note is an introduction to the topic of "second quantization", and hence to quantum "field theory". In the Electromagnetic Interactions note, we have already been exposed to these ideas in our quantization of the electromagnetic field in terms of photons. We develop the concepts more generally here, for both bosons and fermions. One of the uses of this new formalism is that it provides a powerful structure for dealing with the symmetries of the states and operators for systems with many identical particles.

2 Creation and Annihilation Operators

We begin with the idea that emerged in our quantization of the electromagnetic field, and introduce operators that add or remove particles from a system, similar to the changing of excitation quanta of a harmonic oscillator.

To follow an explicit example, suppose that we have a potential well, $V(\mathbf{x})$, with single particle eigenstates $\phi_0(\mathbf{x}), \phi_1(\mathbf{x}), \ldots$ Suppose we have an n (identical) boson system, where all n bosons are in the lowest, ϕ_0, level. Denote this state by $|n\rangle$. We assume that $|n\rangle$ is normalized: $\langle n|n\rangle = 1$. Since the particles are bosons, we can have $n = 0, 1, 2, \ldots$, where $|0\rangle$ is the state with no particles (referred to as the "vacuum").

Now define "annihilation" (or "destruction") operators according to:

$$b_0|n\rangle = \sqrt{n}|n-1\rangle \tag{1}$$

$$b_0^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{2}$$

Note that these operators subtract or add a particle to the system, in the state ϕ_0. They have been defined so that their algebraic properties are identical to the raising/owering operators of the harmonic oscillator. For example, consider the commutator:

$$[b_0, b_0^\dagger]|n\rangle = (b_0 b_0^\dagger - b_0^\dagger b_0)|n\rangle \tag{3}$$

$$= [(n+1) - (n)]\,|n\rangle \tag{4}$$

$$= |n\rangle. \tag{5}$$

Thus $[b_0, b_0^\dagger] = 1$. With these operators, we may write the n-particle state in terms of the vacuum state by:

$$|n\rangle = \frac{(b_0^\dagger)^n}{\sqrt{n!}}|0\rangle. \tag{6}$$

As in the case of the harmonic oscillator, $b_0^\dagger$ is the hermitian conjugate of b_0. To see this, consider the following: We have $b_0^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$. Thus,

$$\langle n+1|b_0^\dagger|n\rangle = \sqrt{n+1}, \tag{7}$$

and hence, $\langle n+1|b_0^\dagger = \sqrt{n+1}\langle n|$, or

$$\langle n|b_0^\dagger = \sqrt{n}\langle n-1|. \tag{8}$$

Likewise, b_0 acts as a creation operator when acting to the left:

$$\langle n|b_0 = \sqrt{n+1}\langle n+1|. \tag{9}$$

We may write the n-particle state in terms of the vacuum state by:

$$|n\rangle = \frac{(b_0^\dagger)^n}{\sqrt{n!}}|0\rangle. \tag{10}$$

Finally, we have the "number of particles" operator: $B_0 \equiv b_0^\dagger b_0$, with

$$B_0|n\rangle = n|n\rangle. \tag{11}$$

Now suppose that the particles are fermions, and define fermion annihilation and creation operators:

$$f_0|1\rangle = |0\rangle, \qquad f_0|0\rangle = 0; \tag{12}$$

$$f_0^\dagger|1\rangle = 0, \qquad f_0^\dagger|0\rangle = |1\rangle. \tag{13}$$

In the $|0\rangle, |1\rangle$ basis, these operators are the 2×2 matrices:

$$f_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad f_0^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{14}$$

With this explicit representation, we see that they are hermitian conjugate to each other. By construction, we cannot put two fermions in the same state with these operators.

The algebraic properties of the fermion operators are different from those of the boson operators. The commutator, in the $|0\rangle, |1\rangle$ basis, is

$$[f_0, f_0^\dagger] = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \neq I. \tag{15}$$

Consider the anticommutator:

$$\begin{aligned} \{f_0, f_0^\dagger\}|1\rangle &= (f_0 f_0^\dagger + f_0^\dagger f_0)|1\rangle = |1\rangle, & (16) \\ \{f_0, f_0^\dagger\}|0\rangle &= |0\rangle & (17) \end{aligned}$$

That is, $\{f_0, f_0^\dagger\} = 1$. Also,

$$\begin{aligned} \{f_0, f_0\} &= 0, & (18) \\ \{f_0^\dagger, f_0^\dagger\} &= 0. & (19) \end{aligned}$$

The number of particles operator is $F_0 = f_0^\dagger f_0$.

Now return to bosons, and consider two levels, ϕ_0 and ϕ_1. Let $|n_0, n_1\rangle$ be the state with n_0 bosons in ϕ_0 and n_1 bosons in ϕ_1. As before, define,

$$\begin{aligned} b_0|n_0, n_1\rangle &= \sqrt{n_0}|n_0 - 1, n_1\rangle & (20) \\ b_0^\dagger|n_0, n_1\rangle &= \sqrt{n_0 + 1}|n_0 + 1, n_1\rangle, & (21) \end{aligned}$$

and also,

$$\begin{aligned} b_1|n_0, n_1\rangle &= \sqrt{n_1}|n_0, n_1 - 1\rangle & (22) \\ b_1^\dagger|n_0, n_1\rangle &= \sqrt{n_1 + 1}|n_0, n_1 + 1\rangle. & (23) \end{aligned}$$

In addition to the earlier commutation relations, we have that the annihilation and creation operators for different levels commute with each other:

$$\begin{aligned} [b_0, b_1] &= 0; \qquad [b_0^\dagger, b_1] = 0 & (24) \\ \left[b_0, b_1^\dagger\right] &= 0; \qquad [b_0^\dagger, b_1^\dagger] = 0 & (25) \end{aligned}$$

We can construct an arbitrary state from the vacuum by:

$$|n_0, n_1\rangle = \frac{(b_0^\dagger)^{n_0}}{\sqrt{n_0!}} \frac{(b_1^\dagger)^{n_1}}{\sqrt{n_1!}} |0, 0\rangle \tag{26}$$

The total number operator is now

$$B = B_0 + B_1 = b_0^\dagger b_0 + b_1^\dagger b_1, \tag{27}$$

so that

$$B|n_0, n_1\rangle = (n_0 + n_1)|n_0, n_1\rangle. \tag{28}$$

In the case of fermions, we now have four possible states: $|0,0\rangle, |1,0\rangle, |0,1\rangle$, and $|1,1\rangle$. We define:

$$\begin{aligned}
f_0^\dagger|0,0\rangle &= |1,0\rangle; \quad f_0^\dagger|1,0\rangle = 0, && (29)\\
f_0|1,0\rangle &= |0,0\rangle; \quad f_0|0,0\rangle = 0, && (30)\\
f_0|0,1\rangle &= 0; \quad f_0^\dagger|1,1\rangle = 0, && (31)\\
f_1^\dagger|0,0\rangle &= |0,1\rangle; \quad f_1|0,0\rangle = f_1|1,0\rangle = 0, && (32)\\
f_1^\dagger|1,0\rangle &= |1,1\rangle; \quad f_1|0,1\rangle = |0,0\rangle, && (33)\\
f_1^\dagger|0,1\rangle &= f_1^\dagger|1,1\rangle = 0; \quad f_1|1,1\rangle = |1,0\rangle. && (34)
\end{aligned}$$

But we must be careful in writing down the remaining actions, of $f_0, f_0^\dagger$ on the states with $n_1 = 1$. These actions are constrained by consistency with the exclusion principle. We must get a sign change if we interchange the two fermions in a state. Thus, consider using the f and $f^\dagger$ operators to "interchange" the two fermions in the $|1,1\rangle$ state: First, take the fermion away from ϕ_1,

$$|1,1\rangle \to |1,0\rangle = f_1|1,1\rangle. \tag{35}$$

Then "move" the other fermion from ϕ_0 to ϕ_1,

$$|1,0\rangle \to |0,1\rangle = f_1^\dagger f_0|1,0\rangle. \tag{36}$$

Finally, restore the other one to ϕ_0,

$$|0,1\rangle \to f_0^\dagger|0,1\rangle = f_0^\dagger f_1^\dagger f_0 f_1|1,1\rangle \tag{37}$$

We require the result to be a sign change, *i.e.*,

$$f_0^\dagger|0,1\rangle = -|1,1\rangle. \tag{38}$$

Since f_0 is the hermitian conjugate of $f_0^\dagger$, we also have $f_0|1,1\rangle = -|0,1\rangle$.

We therefore have the anticommutation relations:

$$\{f_0, f_0^\dagger\} = \{f_1, f_1^\dagger\} = 1. \tag{39}$$

All other anticommutators are zero, including $\{f_0, f_1\} = \{f_0, f_1^\dagger\} = 0$, following from the antisymmetry of fermion states under interchange.

We may generalize these results to spaces with an arbitrary number of single particle states. Thus, let $|n_0, n_1, \ldots\rangle$ be a vector in such a space. For the case of bosons, we have, in general:

$$
\begin{aligned}
[b_i, b_j^\dagger] &= \delta_{ij}, && (40)\\
[b_i, b_j] &= [b_i^\dagger, b_j^\dagger] = 0, && (41)\\
|n_0, n_1, \ldots\rangle &= \cdots \frac{(b_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(b_0^\dagger)^{n_0}}{\sqrt{n_0!}} |0\rangle, && (42)
\end{aligned}
$$

where $|0\rangle$ represents the vacuum state, with all $n_i = 0$. Note that these are the same as the photon annihilation and creation operators $\hat{A}^\dagger, \hat{A}$, that we defined in the Electromagnetic Interactions note, except for the $\sqrt{2\pi/\omega}$ factor.

For the fermion case, we have the generalization:

$$
\begin{aligned}
\{f_i, f_j^\dagger\} &= \delta_{ij}, && (43)\\
\{f_i, f_j\} &= \{f_i^\dagger, f_j^\dagger\} = 0, && (44)\\
|n_0, n_1, \ldots\rangle &= \cdots (f_1^\dagger)^{n_1} (f_0^\dagger)^{n_0} |0\rangle. && (45)
\end{aligned}
$$

The number operators are similar in both cases:

$$
\begin{aligned}
B &= \sum B_i = \sum_i b_i^\dagger b_i, && (46)\\
F &= \sum F_i = \sum_i f_i^\dagger f_i, && (47)
\end{aligned}
$$

and $[B_i, B_j] = [F_i, F_j] = 0$.

3 Field Operators

Consider now plane wave states in a box (rectangular volume V, sides $L_i, i = 1, 2, 3$), with periodic boundary conditions:

$$
\phi_{\mathbf{k}}(\mathbf{x}) = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}}, \tag{48}
$$

where $k_i = 2\pi n_j / L_i$, $n_j = 0, \pm 1, \pm 2, \ldots$. The creation operator $a_{\mathbf{k}s}^\dagger$ (a is either b or f, for bosons or fermions, respectively), adds a particle with

momentum $\mathbf{k}$ and spin projection s; the annilation operator $a_{\mathbf{k}s}$ removes one. Note that $\phi_{\mathbf{k}}(\mathbf{x})$ is the amplitude at $\mathbf{x}$ to find a particle added by $a^\dagger_{\mathbf{k}s}$.

Now consider the operator:

$$\psi^\dagger_s(\mathbf{x}) \equiv \sum_{\mathbf{k}} \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} a^\dagger_{\mathbf{k}s}. \tag{49}$$

This operator adds a particle in a superpositon of momentum states with amplitude $\frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}}$, so that the amplitude for finding the particle at $\mathbf{x}'$ added by $\psi^\dagger_s(\mathbf{x})$ is a coherent sum of amplitudes $e^{i\mathbf{k}\cdot\mathbf{x}'}/\sqrt{V}$, with coefficients $e^{-i\mathbf{k}\cdot\mathbf{x}}/\sqrt{V}$. That is, the amplitude at $\mathbf{x}'$ is

$$\sum_{\mathbf{k}} \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} \frac{e^{i\mathbf{k}\cdot\mathbf{x}'}}{\sqrt{V}} = \delta^{(3)}(\mathbf{x}-\mathbf{x}') \tag{50}$$

[by Fourier series expansion of $\delta^{(3)}(\mathbf{x}-\mathbf{x}')$:

$$g(\mathbf{x}') = \frac{1}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}'} \int_V d^3(\mathbf{x}'') e^{-i\mathbf{k}\cdot\mathbf{x}''} g(\mathbf{x}''), \tag{51}$$

with $g(\mathbf{x}') = \delta^{(3)}(\mathbf{x}-\mathbf{x}')$].

The operator $\psi^\dagger_s(\mathbf{x})$ thus adds a particle at $\mathbf{x}$ – it creates a particle at point $\mathbf{x}$ (with spin projection s). Likewise, the operator

$$\psi_s(\mathbf{x}) \equiv \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} a_{\mathbf{k}s} \tag{52}$$

removes a particle at $\mathbf{x}$. The operators $\psi^\dagger_s(\mathbf{x})$ and $\psi_s(\mathbf{x})$ are called "field operators". They have commutation relations following from the commutation relations for the a and $a^\dagger$ operators:

$$\psi_s(\mathbf{x})\psi_{s'}(\mathbf{x}') \pm \psi_{s'}(\mathbf{x}')\psi_s(\mathbf{x}) = 0 \tag{53}$$

$$\psi^\dagger_s(\mathbf{x})\psi^\dagger_{s'}(\mathbf{x}') \pm \psi^\dagger_{s'}(\mathbf{x}')\psi^\dagger_s(\mathbf{x}) = 0, \tag{54}$$

where the upper sign is for fermions, and the lower sign is for bosons. For bosons, adding (or removing) a particle at $\mathbf{x}$ commutes with adding one at $\mathbf{x}'$. For fermions, adding (or removing) a particle at $\mathbf{x}$ anticommutes with

adding one at $\mathbf{x}'$. Also,

$$\begin{aligned}
\psi_s(\mathbf{x})\psi^\dagger_{s'}(\mathbf{x}') \pm \psi^\dagger_{s'}(\mathbf{x}')\psi_s(\mathbf{x}) &= \sum_{\mathbf{k},\mathbf{k}'} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}e^{i\mathbf{k}'\cdot\mathbf{x}'}}{V} \begin{cases} \{f_{\mathbf{k}s}, f^\dagger_{\mathbf{k}'s'}\} \\ [b_{\mathbf{k}s}, b^\dagger_{\mathbf{k}'s'}] \end{cases} && (55)\\
&= \sum_{\mathbf{k},\mathbf{k}'} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}e^{i\mathbf{k}'\cdot\mathbf{x}'}}{V}\delta_{\mathbf{k}\mathbf{k}'}\delta_{ss'} && (56)\\
&= \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}'}}{V}\delta_{ss'} && (57)\\
&= \delta(\mathbf{x}-\mathbf{x}')\delta_{ss'}. && (58)
\end{aligned}$$

Thus, adding particles commutes (bosons) or anticommutes (fermions) with removing them, unless it is at the same point and spin projection. If it is at the same point (and spin projection) we may consider the case with no particle originally there – the $\psi^\dagger\psi$ term gives zero, but the $\psi\psi^\dagger$ term does not, since it creates a particle which it then removes.

If we suppress the spin indices, we construct a state with n particles at $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_n$ by:

$$|\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_n\rangle = \frac{1}{\sqrt{n!}}\psi^\dagger(\mathbf{x}_n)\ldots\psi^\dagger(\mathbf{x}_1)|0\rangle. \tag{59}$$

Note that such states form a useful basis for systems of many identical particles, since, by the commutation relations of the $\psi^\dagger$'s, they have the desired symmetry under interchanges of $\mathbf{x}_i$'s.[1] For example, for fermions,

$$\psi^\dagger(\mathbf{x}_2)\psi^\dagger(\mathbf{x}_1) = -\psi^\dagger(\mathbf{x}_1)\psi^\dagger(\mathbf{x}_2) \tag{60}$$

gives

$$|\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3, \ldots, \mathbf{x}_n\rangle = -|\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_n\rangle. \tag{61}$$

Note also that we can add another particle, and automatically maintain the desired symmetry:

$$\psi^\dagger(\mathbf{x})|\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_n\rangle = \sqrt{n+1}|\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_n, \mathbf{x}\rangle. \tag{62}$$

[1] These Hilbert spaces of multiple, variable numbers of particles, are known as Fock spaces.

Now let us evaluate:

$$\begin{aligned}
\psi(\mathbf{x})|\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\ldots,\mathbf{x}_n\rangle &= \frac{1}{\sqrt{n!}}\psi(\mathbf{x})\psi^\dagger(\mathbf{x_n})\ldots\psi^\dagger(\mathbf{x}_1)|0\rangle \\
&= \frac{1}{\sqrt{n!}}\left[\delta^{(3)}(\mathbf{x}-\mathbf{x}_n)\pm\psi^\dagger(\mathbf{x}_n)\psi(\mathbf{x})\right]\psi^\dagger(\mathbf{x}_{n-1})\ldots\psi^\dagger(\mathbf{x}_1)|0\rangle \\
&= \frac{1}{\sqrt{n!}}\Big[\delta^{(3)}(\mathbf{x}-\mathbf{x}_n)|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_{n-1}\rangle \\
&\quad \pm\delta^{(3)}(\mathbf{x}-\mathbf{x}_{n-1})|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_{n-2},\mathbf{x}_n\rangle \\
&\quad +\ldots+ \\
&\quad (\pm)^{n-1}\delta^{(3)}(\mathbf{x}-\mathbf{x}_1)|\mathbf{x}_2,\mathbf{x}_2,\ldots,\mathbf{x}_n\rangle\Big], \qquad (63)
\end{aligned}$$

where the upper sign is for bosons and the lower for fermions. This quantity is non-zero if and only if $\mathbf{x}=\mathbf{x}_j$ (and the corresponding suppressed spin projections are also the same). If this is the case, the $n-1$ particle state which remains after performing the operation has the correct symmetry.

Note that

$$\begin{aligned}
\langle\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n| &= \frac{1}{\sqrt{n!}}\left[\psi^\dagger(\mathbf{x}_n)\psi^\dagger(\mathbf{x}_{n-1})\ldots\psi^\dagger(\mathbf{x}_1)|0\rangle\right]^\dagger \\
&= \langle 0|\psi(\mathbf{x}_1)\ldots\psi(\mathbf{x}_n)\frac{1}{\sqrt{n!}}. \qquad (64)
\end{aligned}$$

Thus, by iterating the above repeated commutation process we calculate:

$$\langle\mathbf{x}'_1,\mathbf{x}'_2,\ldots,\mathbf{x}'_n|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n\rangle=\delta_{nn'}\sum_P(\pm)^P P\left[\delta(\mathbf{x}_1-\mathbf{x}'_1)\delta(\mathbf{x}_2-\mathbf{x}'_2)\ldots\delta(\mathbf{x}_n-\mathbf{x}'_n)\right], \qquad (65)$$

where $\sum_P$ is a sum over all permutations, P, of $\mathbf{x}'_1,\mathbf{x}'_2,\ldots,\mathbf{x}'_n$ and the $(-)^P$ factor for fermions inserts a minus sign for odd permutations.

Suppose we wish to create an n particle state $\phi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n)$ which has the desired symmetry, even if ϕ itself does not. The desired state is:

$$|\Phi\rangle=\int d^3(\mathbf{x}_1)\ldots d^3(\mathbf{x}_n)\phi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n)|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n\rangle. \qquad (66)$$

We can calculate the amplitude for observing the particles at $\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n$ by:

$$\begin{aligned}
\langle\mathbf{x}'_1,\mathbf{x}'_2,\ldots,\mathbf{x}'_n|\Phi\rangle &= \int d^3(\mathbf{x}_1)\ldots d^3(\mathbf{x}_n)\phi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n)\langle\mathbf{x}'_1,\mathbf{x}'_2,\ldots,\mathbf{x}'_n|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n\rangle \\
&= \frac{1}{n!}\sum_P(\pm)^P P\phi(\mathbf{x}'_1,\mathbf{x}'_2,\ldots,\mathbf{x}'_n). \qquad (67)
\end{aligned}$$

That is, $\langle \mathbf{x}'_1, \mathbf{x}'_2, \ldots, \mathbf{x}'_n | \Phi \rangle$ is properly symmetrized. If ϕ is already properly symmetrized, then all $n!$ terms in $\sum_P$ are equal and $\langle \mathbf{x}'_1, \mathbf{x}'_2, \ldots, \mathbf{x}'_n | \Phi \rangle = \phi(\mathbf{x}'_1, \mathbf{x}'_2, \ldots, \mathbf{x}'_n)$. If ϕ is normalized to one, and symmetrized, we have:

$$\begin{aligned}
\langle \Phi | \Phi \rangle &= \int d^3(\mathbf{x}_1) \ldots d^3(\mathbf{x}_n) \phi^*(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x_n}) \langle \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x_n} | \\
&\quad \int d^3(\mathbf{x}'_1) \ldots d^3(\mathbf{x}'_n) \phi(\mathbf{x}'_1, \mathbf{x}'_2, \ldots, \mathbf{x}'_n) | \mathbf{x}'_1, \mathbf{x}'_2, \ldots, \mathbf{x}'_n \rangle \\
&= \int d^3(\mathbf{x}_1) \ldots d^3(\mathbf{x}_n) \int d^3(\mathbf{x}'_1) \ldots d^3(\mathbf{x}'_n) \\
&\quad \phi^*(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x_n}) \phi(\mathbf{x}'_1, \mathbf{x}'_2, \ldots, \mathbf{x}'_n) \frac{1}{n!} \sum_P (\pm)^P P \left[\delta(\mathbf{x}_1 - \mathbf{x}'_1) \delta(\mathbf{x}_2 - \mathbf{x}'_2) \ldots \delta(\mathbf{x}_n - \mathbf{x}'_n) \right] \\
&= \int d^3(\mathbf{x}_1) \ldots d^3(\mathbf{x}_n) |\phi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x_n})|^2 && (68) \\
&= 1. && (69)
\end{aligned}$$

We may write the state $|\Phi\rangle$ in terms of an expansion in the amplitudes $\langle \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n | \Phi \rangle$ for observing the particles at $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$:

$$|\Phi\rangle = \int d^3(\mathbf{x}_1) \ldots d^3(\mathbf{x}_n) |\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\rangle \langle \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n | \Phi \rangle. \tag{70}$$

That is, we have the identity operator on symmetrized n particle states:

$$I_n = \int d^3(\mathbf{x}_1) \ldots d^3(\mathbf{x}_n) |\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\rangle \langle \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n |. \tag{71}$$

If $|\Phi\rangle$ is an n particle state, then

$$I_{n'} |\Phi\rangle = \delta_{nn'} |\Phi\rangle. \tag{72}$$

Summing the n particle identity operators gives the identity on the symmetrized states of any number of particles: $I = \sum_{n=0}^{\infty} I_n$, where $I_0 = |0\rangle\langle 0|$.

4 Exercises

1. Consider a two-level fermion system. With respect to basis $|0,0\rangle, |0,1\rangle, |1,0\rangle, |1,1\rangle$, construct the explisict 4×4 matrices representing the creation and annihilation operators $f_0, f_1, f_0^\dagger, f_1^\dagger$. Check that the desired anticommutation relations are satisfied. Form the explicit matrix representation of the total number operator.

2. You showed in Exercise 1 of the Electromagnetic Interactions course note that under a gauge transformation:

$$\mathbf{A}(\mathbf{x},t) \rightarrow \mathbf{A}'(\mathbf{x},t) = \mathbf{A}(\mathbf{x},t) + \nabla\chi(\mathbf{x},t) \tag{73}$$

$$\Phi(\mathbf{x},t) \rightarrow \Phi'(\mathbf{x},t) = \Phi(\mathbf{x},t) - \partial_t\chi(\mathbf{x},t), \tag{74}$$

that the wave function (the solution to the Schrödinger equation) has the corresponding transformation:

$$\psi'(\mathbf{x},t) = e^{iq\chi(\mathbf{x},t)}\psi(\mathbf{x},t). \tag{75}$$

Generalize this result to the case of an N particle system.

SECOND QUANTIZATION

Lecture notes with course Quantum Theory

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Fall 2008

SECOND QUANTIZATION

Second Quantization

1. Introduction and history

Second quantization is the standard formulation of *quantum many-particle theory.* It is important for use both in *Quantum Field Theory* (because a quantized field is a qm operator with *many degrees of freedom*) and in *(Quantum) Condensed Matter Theory* (since matter involves *many particles*).

Identical (= indistinguishable) particles $\longrightarrow$ state of two particles must either be symmetric or anti-symmetric under exchange of the particles.

$$|a \otimes b\rangle_B = \frac{1}{\sqrt{2}} \left(|a_1 \otimes b_2\rangle + |a_2 \otimes b_1\rangle \right) \qquad \text{bosons; symmetric} \tag{1a}$$

$$|a \otimes b\rangle_F = \frac{1}{\sqrt{2}} \left(|a_1 \otimes b_2\rangle - |a_2 \otimes b_1\rangle \right) \qquad \text{fermions; anti} - \text{symmetric} \tag{1b}$$

Motivation: why do we need the "second quantization formalism"?

(a) for practical reasons: computing matrix elements between N-particle symmetrized wave functions involves $(N!)^2$ terms (integrals); see the symmetrized states below.

(b) it will be extremely useful to have a formalism that can handle a non-fixed particle number N, as in the grand-canonical ensemble in Statistical Physics; especially if you want to describe processes in which particles are created and annihilated (as in typical high-energy physics accelerator experiments). So: both for Condensed Matter and High-Energy Physics this formalism is crucial!

(c) To describe interactions the formalism to be introduced will be vastly superior to the wave-function- and Hilbert-space-descriptions.

Some historical remarks

1927: Dirac - Field theory of the electromagnetic field using *creation and annihilation operators.*
1927: Jordan & Klein and 1928: Jordan & Wigner - Note that Dirac's description is also useful for many-particle systems in which particles may interact (!).
1932: Fock - Invented *Fock space*
For more history see an article in *Physics Today*, Oct.'99, about Pascual Jordan (1902-1980; who never received a Nobel prize; Dirac received his in 1933, Wigner in 1963).

The spin-statistics theorem: Particles of integer spin $(0, \hbar, 2\hbar, \ldots)$ are bosons, particles of half-integer spin $(\hbar/2, 3\hbar/2, 5\hbar/2, \ldots)$ are fermions.
The proof of this theorem needs the *relativistic theory of quantized field* and is beyond the scope of this course. Also: the proof is very complicated, which is unfortunate for such a fundamental, important result of theoretical physics.

2. The N-boson system

One-boson Hilbert space $\mathcal{E}_1$

complete set of physical properties $\hat{k}$; quantum numbers k;
basis: $\{|k\rangle\}$.

N bosons: product space: $\mathcal{E}_N = \mathcal{E}_1^{(1)} \otimes \mathcal{E}_1^{(2)} \otimes \cdots \otimes \mathcal{E}_1^{(N)}$
basis states: $|k_1^{(1)} k_2^{(2)} \ldots k_N^{(N)}\rangle$
(Note: all k_i can take on all values in $\hat{k}$-spectrum)

Subspace of fully symmetrized states: $\mathcal{E}_N^{(s)}$

$$|k_1 \ldots k_N\rangle \equiv \hat{S}|k_1^{(1)} k_2^{(2)} \ldots k_N^{(N)}\rangle = \frac{1}{N!} \sum_P |k_{P1}^{(1)} k_{P2}^{(2)} \ldots k_{PN}^{(N)}\rangle \tag{2}$$

$\hat{S}$ is the symmetrization operator, working on a general N-particle state.
The set of symmetrized states is complete:

$$\textit{completeness} \qquad \sum_{k_1 \ldots k_N} |k_1 \ldots k_N\rangle\langle k_1 \ldots k_N| = \hat{1} \quad \text{in} \quad \mathcal{E}_N^{(s)} \ , \tag{3}$$

but <u>not</u> normalized(!):

$$\langle k_1 \ldots k_N | k_1' \ldots k_N'\rangle = \frac{1}{N!} \sum_P \delta(k_{P1}, k_1')\delta(k_{P2}, k_2') \ldots \delta(k_{PN}, k_N') \tag{4}$$

Notation: In formula (3) and in the following sums over k should be read as integrals over k in case the spectrum of $\hat{k}$ is continuous. Even though a sum is written the formulae should be understood as covering both the cases of discrete and continuous spectra.

Remark: The symmetrized states are not orthonormal because the RHS (right-hand side) of (4) will in general be smaller than 1, i.e. the basis vectors are *shorter* than 1.

$\hat{k}$-spectrum: $\{a, b, c, \ldots\}$
occupation numbers: $n_a, n_b, n_c, \ldots$ with $\sum_k n_k = N$
Notation for state in **occupation number representation**: $\{n_a, n_b, n_c, \ldots; N\} \equiv \{n_k; N\}$

<u>Orthonormalized, complete set of states</u>:

$$\big|\{n_k; N\}\rangle \equiv |n_a, n_b, \ldots; N\rangle = \left(\frac{N!}{\prod_k n_k!}\right)^{\frac{1}{2}} |k_1 \ldots k_N\rangle \tag{5}$$

NB: This only works for a discrete spectrum! (for obvious reasons). One can show orthonormality and completeness for these states:

$$\textit{orthonormality} \qquad \langle\{n_k;N\}|\{n'_k;N\}\rangle = \prod_k \delta_{n_k n'_k} \tag{6}$$

$$\textit{completeness} \qquad \sum_{\{n_k;N\}} \Big|\{n_k;N\}\rangle\langle\{n_k;N\}\Big| = \hat{1} \quad \text{in} \quad \mathcal{E}_N^{(s)} \ , \tag{7}$$

For ease of notation and because it works for both discrete **and** continuous spectra, we will work with the (non-orthonormal) symmetrized basis $\{|k_1 \dots k_N\rangle\}$ in the following.
Physical properties for the N-boson system:
one-body operator:

$$\hat{F}_N = \sum_i \hat{f}^{(i)} \ , \tag{8}$$

where $\hat{f}^{(i)}$ is a one-particle operator, e.g. $\hat{p}^2/2m$.
two-body operator:

$$\hat{G}_N = \tfrac{1}{2}\sum_{i\neq j} \hat{g}^{(i,j)} \ , \tag{9}$$

with $\hat{g}^{(i,j)} = \hat{g}^{(j,i)}$ a two-particle operator, e.g. $V\left(|\hat{\vec{r}}_i - \hat{\vec{r}}_j|\right)$.
In the k-representation in $\mathcal{E}_N^{(s)}$ the operators $\hat{F}_N$ and $\hat{G}_N$ take the form:

$$\hat{F}_N = N \sum_{k_1 k'_1} \sum_{k_2 \dots k_N} |k_1 k_2 \dots k_N\rangle f(k_1,k'_1)\langle k'_1 k_2 \dots k_N| \tag{10}$$

with $f(k_1,k'_1) \equiv \langle k_1|\hat{f}^{(1)}|k'_1\rangle$. Similarly:

$$\hat{G}_N = \frac{N(N-1)}{2} \sum_{k_1 k'_1 k_2 k'_2} \sum_{k_3 \dots k_N} |k_1 k_2 k_3 \dots k_N\rangle g(k_1,k_2;k'_1,k'_2)\langle k'_1 k'_2 k_3 \dots k_N| \tag{11}$$

with $g(k_1,k_2;k'_1,k'_2) \equiv \langle k_1^{(1)} k_2^{(2)}|\hat{g}^{(1,2)}|k_1'^{(1)} k_2'^{(2)}\rangle$.

Note that because of the use of symmetrized states and the symmetric form of the operators $\hat{F}_N$ and $\hat{G}_N$, these operators can be expressed in terms of matrix elements of one- and two-body operators between one- and two-particle states, respectively.

In this section, we have been concerned with the complication of the requirement of symmetrization, in the next section we will tackle the unifying description for an arbitrary number of particles, which is the actual purpose of the formalism.

3. The many-boson system

a. "The big picture"

a1. Fock space

$$\mathcal{E} = \mathcal{E}_0 \oplus \mathcal{E}_1 \oplus \mathcal{E}_2^{(s)} \oplus \mathcal{E}_3^{(s)} \oplus \cdots \tag{12}$$

The space $\mathcal{E}_0$ consists of only one state: the *vacuum* state: $|0\rangle$.
A linear operator $\hat{A}$ on $\mathcal{E}$ is represented as a *very big* matrix, which can be subdivided into (N,N')-blocks, with N,N' the corresponding fixed-particle-number subspaces of $\mathcal{E}$.

a2. Creation- and annihilation-operators

Creation- and annihilation-operators $\hat{a}^\dagger(k)$ and $\hat{a}(k)$ will be introduced. These will have non-zero matrix elements only in (N, N') blocks which differ by one in particle number.

a3. Many-body operators $\hat{O}$

All many-body operators can be expressed in the fundamental operators, the creation- and annihilation-operators.
Example: The Bose-Hubbard model (or: boson Hubbard model)

$$\hat{H}_{\mathrm{BH}} = -\sum_{\langle i,j\rangle} t_{ij}\left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i\right) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \tag{13}$$

where $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the number operator, counting the number of bosons on site i of a lattice. There will be an interaction energy U if there are two bosons on a site. The first term is a *hopping* term for bosons hopping between neighboring sites j and i.

b. "Details" (getting specific)

b1. Creation- and annihilation-operators

Definition of <u>creation operator</u>:

$$\hat{a}^\dagger(k)|0\rangle = |k\rangle \tag{14a}$$

$$\hat{a}^\dagger(k)|k_1 \dots k_N\rangle = \sqrt{N+1}\,|kk_1 \dots k_N\rangle \tag{14b}$$

Therefore:

$$|k_1 \dots k_N\rangle = \frac{1}{\sqrt{N!}}\hat{a}^\dagger(k_1)\dots\hat{a}^\dagger(k_N)|0\rangle \tag{15}$$

<u>Matrix for $\hat{a}^\dagger(k)$</u>: From this definition for $\hat{a}^\dagger(k)$ one can derive the matrix elements of $\hat{a}^\dagger(k)$ in Fock space: (take $N' = N - 1$)

$$\langle k_1 \dots k_N|\hat{a}^\dagger(k)|k_1' \dots k_{N-1}'\rangle = \sqrt{N}\langle k_1 \dots k_N|kk_1' \dots k_{N-1}'\rangle$$

$$= \frac{\sqrt{N}}{N!}\sum_P \delta(k_{P1}, k)\delta(k_{P2}, k_1')\dots\delta(k_{PN}, k_{N-1}')$$

$$= \frac{\sqrt{N}}{N!}(N-1)!\left\{\delta(k_1, k)\langle k_2 \dots k_N|k_1' \dots k_{N-1}'\rangle + \delta(k_2, k)\langle k_1 k_3 \dots k_N|k_1' \dots k_{N-1}'\rangle + \cdots\right\}$$

$$= \frac{1}{\sqrt{N}}\left\{\sum_{i=1}^{N}\delta(k_i, k)\langle k_1 \dots k_{i-1}k_{i+1} \dots k_N|\right\} k_1' \dots k_{N-1}'\rangle \tag{16}$$

In the first two steps we have used equations (14b) and (4), respectively. In the third step, we split the sum over permutations ($N!$ terms) into N sums with $(N-1)!$ terms each, in which the first sum is over all permutations with $P1 = 1$, the second sum over all permutations with $P1 = 2$, etc. In the second term, $P2$ to PN then take values $1, 3, \dots N$. In the last step, the expression is written more compactly.

Matrix for $\hat{a}(k)$: Now the matrix elements of $\hat{a}(k)$ are easily derived by making use of: $\overline{\langle\omega'|\hat{a}|\omega\rangle} = \langle\omega|\hat{a}^\dagger|\omega'\rangle^\star$. For the $(N, N' = N+1)$ block we find:

$$\langle k'_1 \dots k'_{N-1}|\hat{a}(k)|k_1 \dots k_N\rangle = \langle k_1 \dots k_N|\hat{a}^\dagger(k)|k'_1 \dots k'_{N-1}\rangle^\star =$$

$$= \langle k'_1 \dots k'_{N-1}| \left\{ \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \delta(k_i, k)|k_1 \dots k_{i-1}k_{i+1} \dots k_N\rangle \right\} , \qquad (17)$$

from which it follows how $\hat{a}(k)$ operates in Fock space :

$$\hat{a}(k)|0\rangle = 0 \qquad (18a)$$

$$\hat{a}(k)|k_1 \dots k_N\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \delta(k, k_i)|k_1 \dots k_{i-1}k_{i+1} \dots k_N\rangle \qquad (18b)$$

Note that (18b) is more complicated than the lowering operator for the simple harmonic oscillator, $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$, because there is more choice in what to lower/annihilate. If all k_i equal k, one recovers a similar result as for the simple harmonic oscillator.

It is important to note that (14a) implies:

$$\langle k| = \langle 0|\hat{a}(k) \qquad (19)$$

(therefore the annihilation operator working to the left acts as a creation operator; these names are therefore just a convention!)

b2. Commutation relations

From the results in section b1. the fundamental algebraic relations, i.e. the commutation relations, between the $\hat{a}^\dagger(k)$ and $\hat{a}(k)$ follow directly (work this out for yourself!):

$$\left[\hat{a}^\dagger(k), \hat{a}^\dagger(\ell)\right] = \hat{0} \qquad (20a)$$

$$[\hat{a}(k), \hat{a}(\ell)] = \hat{0} \qquad (20b)$$

$$\left[\hat{a}(k), \hat{a}^\dagger(\ell)\right] = \delta(k, \ell)\,\hat{1} \qquad (20c)$$

NB1: The commutation relation (20c) only takes on this elegant form because of the **factor** $\sqrt{N+1}$ in the definition of $\hat{a}^\dagger(k)$, (14b).

NB2: The commutation relations (20) are now just as we saw them for **phonons** and **independent harmonic oscillators** before.

NB3: The commutation relations are a **consequence of symmetry**! Note that the same in a certain sense is true for the canonical commutation relation $[X, P] = \hbar i\hat{1}$ (see Ch. 8 of Le Bellac).

b3. Many-body operators $\hat{F}$ and $\hat{G}$ in Fock space

$$\hat{F} = \sum_{N=1}^{\infty} \hat{F}_N = \sum_{N=1}^{\infty} \sum_i \hat{f}^{(i)} \tag{21}$$

Now use:

$$|k_1\rangle\langle k_1'| = \hat{a}^\dagger(k_1)|0\rangle\langle 0|\hat{a}(k_1') \tag{22}$$

and:

$$N|k_1 k_2 \ldots k_N\rangle\langle k_1' k_2 \ldots k_N| = \hat{a}^\dagger(k_1)|k_2 \ldots k_N\rangle\langle k_2 \ldots k_N|\hat{a}(k_1') \tag{23}$$

Using formula (10), $\hat{F}$ is found to be:

$$\hat{F} = \sum_{k_1,k_1'} \hat{a}^\dagger(k_1) f(k_1,k_1') \left[|0\rangle\langle 0| + \sum_{k_2} |k_2\rangle\langle k_2| + \cdots \right] \hat{a}(k_1') \tag{24}$$

The expression between the large brackets [,] is precisely the identity in $\mathcal{E}$, because of the completeness of the basis of symmetrized states in $\mathcal{E}_N^{(s)}$. The final result for the general form of a many-body operator constructed from one-particle operators in the second quantization formalism therefore is:

$$\hat{F} = \sum_{k_1,k_1'} \hat{a}^\dagger(k_1) f(k_1,k_1') \hat{a}(k_1') \tag{25}$$

Using more ink and formula (11), but completely analogously (*peeling off* two k's) one derives the general form for the many-body operator constructed from two-particle operators:

$$\hat{G} = \tfrac{1}{2} \sum_{k_1,k_2,k_1',k_2'} \hat{a}^\dagger(k_1)\hat{a}^\dagger(k_2) g(k_1,k_2;k_1',k_2') \hat{a}(k_2')\hat{a}(k_1') \tag{26}$$

4. Identical spin-0 particles

Application of the preceding: form of operators in *Second Quantization* for identical particles with mass m and spin 0 (bosons!).

<u>Discrete $\vec{k}$-representation</u>

In $\mathcal{E}_1$: $\hat{\vec{k}}$-basis: $\left\{|\vec{k}\rangle\right\}$

discrete $\Leftrightarrow$ periodicity volume $V = L^3$

$\vec{k} = \frac{2\pi}{L}\vec{n}$ with n_x, n_y, n_z integer numbers.

The creation- and annihilation-operators are written as: $\hat{a}_{\vec{k}}^\dagger$ and $\hat{a}_{\vec{k}}$

a. What is the form of many-body operators $\hat{F}$?

General procedure: (i) determine matrix elements

$$f(\vec{k},\vec{k}') = \langle\vec{k}|\hat{f}^{(1)}|\vec{k}'\rangle \tag{27}$$

(ii) Using (i):

$$\hat{F} = \sum_{\vec{k},\vec{k}'} \hat{a}^\dagger_{\vec{k}} f(\vec{k},\vec{k}') \hat{a}_{\vec{k}'} \tag{28}$$

<u>Examples</u>

1. $\hat{f} = |\vec{k}\rangle\langle\vec{k}| \quad \longrightarrow \quad f(\vec{k}',\vec{k}'') = \langle\vec{k}'|\vec{k}\rangle\langle\vec{k}|\vec{k}''\rangle = \delta_{\vec{k}',\vec{k}}\delta_{\vec{k},\vec{k}''} \quad \longrightarrow$

$$\hat{F} = \sum_{\vec{k}',\vec{k}''} \hat{a}^\dagger_{\vec{k}'}\, \delta_{\vec{k}',\vec{k}}\, \delta_{\vec{k},\vec{k}''}\, \hat{a}_{\vec{k}''} = \hat{a}^\dagger_{\vec{k}}\, \hat{a}_{\vec{k}} \equiv \hat{n}_{\vec{k}} \tag{29}$$

operator: **number of particles with wave vector** $\vec{k}$

2. $\hat{f} = \hat{1} \quad \longrightarrow \quad$ (Use 1. and $\hat{1} = \sum_{\vec{k}} |\vec{k}\rangle\langle\vec{k}|$)

$$\hat{F} = \sum_{\vec{k}} \hat{n}_{\vec{k}} \equiv \hat{N} \tag{30}$$

operator: **total particle number**

3. $\hat{f} = \frac{\hat{\vec{p}}^2}{2m} \quad \longrightarrow \quad f(\vec{k},\vec{k}') = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)\, \delta_{\vec{k},\vec{k}'}$

$$\hat{F} = \cdots = \sum_{\vec{k}} \varepsilon_k\, \hat{n}_{\vec{k}} \equiv \hat{H}^{(0)} \tag{31}$$

where $\varepsilon_k \equiv \hbar^2 k^2/2m$.
operator: **kinetic energy of many-boson system**

4. (Non-diagonal in $\vec{k}$-representation) external potential $u(\vec{r})$

To compute the necessary $(\vec{k},\vec{k}')$ matrix element it is convenient to switch to the $\vec{r}$-representation (insert two complete sets of states):

$$\langle\vec{k}|u(\vec{r})|\vec{k}'\rangle = \int_V d\vec{r} \int_V d\vec{r}'\, \langle\vec{k}\,|\vec{r}\rangle\langle\vec{r}\,|u(\vec{r})|\vec{r}\,'\rangle\langle\vec{r}\,'\,|\vec{k}'\rangle$$

with:

$$\langle\vec{r}\,|\vec{k}\rangle = \frac{1}{\sqrt{V}}\, e^{i\vec{k}\cdot\vec{r}} \qquad (\star)$$

and use that

$$\int_V d\vec{r}\,|\vec{r}\rangle\langle\vec{r}\,| = \hat{1}$$

Defining the Fourier components, c.q. transform, as follows:

$$u_{\vec{q}} = \frac{1}{\sqrt{V}} \int_V d\vec{r}\; e^{-i\vec{q}\cdot\vec{r}}\, u(\vec{r}) \tag{32a}$$

(as a result:

$$u(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{q}} u_{\vec{q}}\; e^{i\vec{q}\cdot\vec{r}} \tag{32b}$$

),

one finds (this is one of the problems in Problem Session 6):

$$\hat{F} \longrightarrow \hat{U} = \frac{1}{\sqrt{V}} \sum_{\vec{k},\vec{k}'} \hat{a}^\dagger_{\vec{k}}\, u_{\vec{k}-\vec{k}'}\, \hat{a}_{\vec{k}'} = \sum_{\vec{q}} \frac{u_{\vec{q}}}{\sqrt{V}} \sum_{\vec{k}'} \hat{a}^\dagger_{\vec{k}'+\vec{q}}\, \hat{a}_{\vec{k}'} \tag{33}$$

operator: **potential energy of many-boson system**

NB: The Fourier component that appears in the potential energy is the one corresponding to the difference wave vector $\vec{k} - \vec{k}'$ of the two wave vectors of the creation- and annihilation-operators: interaction happens with *conservation of momentum.*

b. Intermezzo: Change of representation and continuous $\vec{k}$-representation

(i) The basic formula for a change of representation is:

$$\hat{a}^\dagger(q) = \sum_k \hat{a}^\dagger(k)\, \langle k|q\rangle \qquad (I.1)$$

It's Hermitian conjugate is:

$$\hat{a}(q) = \sum_k \langle q|k\rangle\, \hat{a}(k) \qquad (I.2)$$

Note that we only need the scalar product $\langle k|q\rangle$ of <u>one-particle</u> basis states to switch representation, even for a description of many-body systems.

The above can be shown very elegantly in Dirac notation, as follows. For the q-representation we have:

$$\hat{a}^\dagger(q)|0\rangle = |q\rangle \qquad (I.3a)$$

$$\hat{a}^\dagger(q)|q_1 \dots q_N\rangle = \sqrt{N+1}|qq_1 \dots q_N\rangle \qquad (I.3b)$$

For one particle we have:

$$|q\rangle = \sum_k |k\rangle\langle k|q\rangle \qquad (I.4)$$

Then, symmetrizing state

$$|q_1^{(1)} \dots q_N^{(N)}\rangle = \sum_{k_1 \dots k_N} |k_1^{(1)} \dots k_N^{(N)}\rangle\langle k_1|q_1\rangle \cdots \langle k_N|q_N\rangle$$

gives:

$$|q_1 \dots q_N\rangle = \sum_{k_1 \dots k_N} |k_1 \dots k_N\rangle\langle k_1|q_1\rangle \cdots \langle k_N|q_N\rangle \qquad (I.5)$$

Now the expression of $\hat{a}^\dagger(q)$ in terms of the $\hat{a}^\dagger(k)$, formula (I.1), follows from:

$$\hat{a}^\dagger(q)|q_1 \dots q_N\rangle = \sqrt{N+1}|qq_1 \dots q_N\rangle =$$

$$= \sqrt{N+1} \sum_{kk_1 \dots k_N} |kk_1 \dots k_N\rangle\langle k|q\rangle\langle k_1|q_1\rangle \cdots \langle k_N|q_N\rangle$$

$$= \sum_{kk_1\ldots k_N} \hat{a}^\dagger(k)|k_1\ldots k_N\rangle\langle k|q\rangle\langle k_1|q_1\rangle\cdots\langle k_N|q_N\rangle$$

$$= \sum_k \hat{a}^\dagger(k)\langle k|q\rangle \left[\sum_{k_1\ldots k_N} |k_1\ldots k_N\rangle\langle k_1|q_1\rangle\cdots\langle k_N|q_N\rangle\right]$$

Because the expression between the big brackets is according to (I.5) precisely $|q_1\ldots q_N\rangle$ and this holds for a general state $|q_1\ldots q_N\rangle$ in Fock space, we have proven the change-of-representation formula (I.1).

(ii) continuous $\vec{k}$-representation: to change from the **discrete** $\vec{k}$-representation to the **continuous** $\vec{k}$-representation one just needs to rescale the state vectors:

$$|\vec{k}\rangle_{\text{continuous}} = \left(\frac{L}{2\pi}\right)^{3/2} |\vec{k}\rangle_{\text{discrete}} = \frac{\sqrt{V}}{(2\pi)^{3/2}}\,|\vec{k}\rangle_{\text{discrete}} \qquad (I.6)$$

This rescaling arises because in the continuum limit, $L \longrightarrow \infty$, sums over discrete $\vec{k}$ turn into integrals over continuous $\vec{k}$ as follows:

$$\frac{1}{L^3}\sum_{\vec{k}}\cdots \qquad \longrightarrow \qquad \int \frac{d\vec{k}}{(2\pi)^3}\cdots \qquad (I.7)$$

(see also section 9.6.2 in Le Bellac). As a result we have:

$$\langle\vec{r}|\vec{k}\rangle_{\text{discrete}} = \frac{1}{\sqrt{V}}\,e^{i\vec{k}\cdot\vec{r}} \qquad \text{and} \qquad \langle\vec{r}|\vec{k}\rangle_{\text{continuous}} = \frac{1}{(2\pi)^{3/2}}\,e^{i\vec{k}\cdot\vec{r}} \qquad (I.8)$$

(This explains the seeming discrepancy between ($\star$) above and (9.21)-(9.22) in Le Bellac). The completeness relations in the two $\vec{k}$-representations then read as we are used to:

$$\sum_{\vec{k}} |\vec{k}\rangle_{d\ d}\langle\vec{k}| = \hat{1} \qquad \text{and} \qquad \int d\vec{k}\ |\vec{k}\rangle_{c\ c}\langle\vec{k}| = \hat{1} \qquad (I.9)$$

(d: discrete, c: continuous).

c. Quantum fields: the $\vec{r}$-representation

Instead of the discrete (or: continuous) $\vec{k}$-representation, one can also present the whole formalism in the (continuous) $\vec{r}$-representation; it is customary to then call the corresponding creation- and annihilation-operators $\hat{\psi}^\dagger(\vec{r})$ and $\hat{\psi}(\vec{r})$. These operators are what we called *quantized fields* before (Ch.11 of Le Bellac). It is important not to confuse these operators with *wave functions*!

According to (I.2) and (I.8) we have:

$$\hat{\psi}(\vec{r}) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\,\hat{a}_{\vec{k}} \qquad (34a)$$

$$\hat{a}_{\vec{k}} = \frac{1}{\sqrt{V}} \int_V d\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\, \hat{\psi}(\vec{r}) \qquad (34b)$$

All many-body operators can be expressed in terms of the $\hat{\psi}^\dagger(\vec{r})$ and $\hat{\psi}(\vec{r})$. This can be done in two ways; (i) starting from a definition of $\hat{\psi}^\dagger(\vec{r})$ and $\hat{\psi}(\vec{r})$ in the $\vec{r}$-representation (just as we did for the discrete $\vec{k}$-representation above), or: (ii) starting from the expressions in the discrete $\vec{k}$-representation and using the "Fourier transform" (34a) and (34b). Some examples of the results are:

$$\hat{N} = \int d\vec{r}\, \hat{\psi}^\dagger(\vec{r})\, \hat{\psi}(\vec{r}) \qquad (35)$$

$$\hat{P} = \int d\vec{r}\, \hat{\psi}^\dagger(\vec{r})\, \frac{\hbar}{i}\frac{\partial}{\partial\vec{r}}\, \hat{\psi}(\vec{r}) \qquad \text{operator: } \textbf{total momentum} \qquad (36)$$

$$\hat{H}^{(0)} = \int d\vec{r}\, \hat{\psi}^\dagger(\vec{r}) \left(-\frac{\hbar^2}{2m}\Delta\right) \hat{\psi}(\vec{r}) \qquad (37)$$

where Δ is the Laplace operator $(= \left(\vec{\nabla}\right)^2)$.

<u>Commutation relations</u>: the following commutation relations can be straightforwardly derived from those for the $\hat{a}^\dagger_{\vec{k}}$ and $\hat{a}_{\vec{k}}$:

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')\right] = 0 \quad , \quad \left[\hat{\psi}^\dagger(\vec{r}), \hat{\psi}^\dagger(\vec{r}\,')\right] = 0 \quad , \quad \left[\hat{\psi}(\vec{r}), \hat{\psi}^\dagger(\vec{r}\,')\right] = \delta(\vec{r}-\vec{r}\,')\,\hat{1} \qquad (38)$$

Since the commutation relations are preserved in the change of representation (34), this change of representation is called a *canonical transformation*.
It is now straightforward to show:

$$\left[\hat{H}^{(0)}, \hat{\psi}(\vec{r})\right] = \frac{\hbar^2}{2m}\Delta\hat{\psi}(\vec{r}) \qquad (39)$$

<u>Dynamics of $\hat{a}^\dagger_{\vec{k}}$ and $\hat{a}_{\vec{k}}$</u>: This is derived in a similar way as in section 11.3.2 of LB (*Quantization of a scalar field in 1D*). For a **free** many-boson system:

$$\frac{d}{dt}\,\hat{a}_{\vec{k}}(t) = \frac{i}{\hbar}\left[\hat{H}^{(0)}, \hat{a}_{\vec{k}}(t)\right] = \frac{i}{\hbar}\sum_{\vec{k}'} \varepsilon_{k'}\, \left[\hat{n}_{\vec{k}'}, \hat{a}_{\vec{k}}(t)\right] = -\frac{i\varepsilon_k}{\hbar}\,\hat{a}_{\vec{k}}(t) \;\longrightarrow\; \hat{a}_{\vec{k}}(t) = \hat{a}_{\vec{k}}\, e^{-i\omega_k t} \quad (40a)$$

where $\omega_k \equiv \varepsilon_k/\hbar$ (the commutator is evaluated in one of the problems). Analogously:

$$\hat{a}^\dagger_{\vec{k}}(t) = \hat{a}^\dagger_{\vec{k}}\, e^{i\omega_k t} \qquad (40b)$$

Having obtained the above results one can understand how the name "second quantization" came about. Let us recall the time-dependent Schrödinger equation for a free particle:

$$i\hbar\frac{\partial}{\partial t}\,\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{r},t) \qquad (41)$$

The general solution is a linear combination of plane waves (as substitution will quickly confirm):

$$\psi(\vec{r},t) = \sum_{\vec{k}} a_{\vec{k}} \frac{e^{i(\vec{k}\cdot\vec{r}-\omega_k t)}}{\sqrt{V}} \tag{42}$$

with $\hbar\omega_k = \varepsilon_k = \hbar^2 k^2/2m$ and the $a_{\vec{k}}$ are Fourier**coefficients** (i.e. numbers!).

For the operators $\hat{\psi}(\vec{r},t)$ (Heisenberg picture) we have, in case of free bosons (using the result (39)):

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\vec{r},t) = -\left[\hat{H}^{(0)}, \hat{\psi}(\vec{r},t)\right] = -\frac{\hbar^2}{2m}\Delta\hat{\psi}(\vec{r},t) \tag{43}$$

Combining (34a) and (40a), we find as a solution:

$$\hat{\psi}(\vec{r},t) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\,\hat{a}_{\vec{k}}(t) = \sum_{\vec{k}} \hat{a}_{\vec{k}} \frac{e^{i(\vec{k}\cdot\vec{r}-\omega_k t)}}{\sqrt{V}} \tag{44}$$

Comparing (43) and (44) with (41) and (42), we see that we get the *quantum theory of many particles* from the *quantum theory of one particle* by replacing the Fourier-coefficients $a_{\vec{k}}, a^*_{\vec{k}}$ by (annihilation-, creation-) operators $\hat{a}_{\vec{k}}, \hat{a}^\dagger_{\vec{k}}$! This procedure is similar as in the case of *quantizing* the classical electromagnetic field (Fourier-coefficients become operators; see also the other examples in Ch.11 LB). This purely formal resemblance of quantization procedures has led to the unfortunate name of "second quantization", which according to some should be banished, but because of it's widespread use probably never will. It is important to stress that there is no such thing as *quantizing twice*: there is only one Quantum Theory!

5. The N-fermion system

One-fermion Hilbert space $\mathcal{E}_1$

complete set of physical properties $\hat{k}$; quantum numbers k; basis: $\{|k\rangle\}$.

Now what k stands for will at least include a spin quantum number σ: e.g. k stands for: $\vec{k}\sigma$ or $\vec{r}\sigma$
N fermions: product space: $\mathcal{E}_N = \mathcal{E}_1^{(1)} \otimes \mathcal{E}_1^{(2)} \otimes \cdots \otimes \mathcal{E}_1^{(N)}$
basis states: $|k_1^{(1)} k_2^{(2)} \ldots k_N^{(N)}\rangle$
(Note: all k_i can take on all values in $\hat{k}$-spectrum)

Subspace of fully **anti**-symmetrized states: $\mathcal{E}_N^{(a)}$

$$|k_1 \ldots k_N\rangle \equiv \hat{A}|k_1^{(1)} k_2^{(2)} \ldots k_N^{(N)}\rangle = \frac{1}{N!}\sum_P \mathrm{sign}(P)|k_{P1}^{(1)} k_{P2}^{(2)} \ldots k_{PN}^{(N)}\rangle \tag{45}$$

Here the anti-symmetrization operator $\hat{A}$ is defined as:

$$\hat{A} \equiv \frac{1}{N!}\sum_P \mathrm{sign}(P)\,\hat{U}_P \tag{46}$$

where $\hat{U}_P$ is the permutation operator and sign(P) denotes the *sign of the permutation*: sign(P) = +1 or -1, depending on whether the permutation consists of an even or odd number of pair exchanges, respectively (any permutation of N entities can be seen as a product of a number of pair exchanges).

As for the N-boson system, the set of anti-symmetrized states $|k_1 \dots k_N\rangle$ is overcomplete and non-orthonormal:

$$\langle k_1 \dots k_N | k'_1 \dots k'_N \rangle = \frac{1}{N!} \sum_P \text{sign}(P) \delta(k_{P1}, k'_1) \delta(k_{P2}, k'_2) \dots \delta(k_{PN}, k'_N) \tag{47}$$

Note the extra factor sign(P) compared to the bosonic case; this factor will make it even harder to reach 1, even if $k_1 = k'_1$, etc.; cf. formula (4).

Operators $\hat{F}_N$ and $\hat{G}_N$ are the same as for bosons, formulae (10) and (11).

Occupation-number representation:

$$\Big| \{n_k; N\} \rangle \equiv |n_a, n_b, \dots; N\rangle \equiv \sqrt{N!}\, |k_1 \dots k_N\rangle \tag{48}$$

The above formula is the analogon of formula (5) for bosons, where we have taken the *Pauli Exclusion Principle* into account, which demands that the state vector changes sign if two particles are interchanged; therefore n_k cannot be larger than 1: $n_k = 0$ or $n_k = 1$. For fermions the order is important (to determine the overall sign of the state vector); we will typically assume: $k_1 < k_2 < k_3 < \dots < k_N$. In case k is shorthand for more quantum numbers, one has to agree on a more general convention to order the one-particle states, but this can always be done.

6. The many-fermion system

a. Fock space

$$\mathcal{E} = \mathcal{E}_0 \oplus \mathcal{E}_1 \oplus \mathcal{E}_2^{(a)} \oplus \mathcal{E}_3^{(a)} \oplus \cdots \tag{49}$$

Again the space $\mathcal{E}_0$ consists of only one state: the *vacuum* state: $|0\rangle$.

b. Creation- and annihilation operators

Definition of creation operator:

$$\hat{a}^\dagger(k)|0\rangle = |k\rangle \tag{50a}$$

$$\hat{a}^\dagger(k)|k_1 \dots k_N\rangle = \sqrt{N+1}\, |k k_1 \dots k_N\rangle \tag{50b}$$

Using

$$\langle \gamma | \hat{a}^\dagger(k) | \delta \rangle^* = \langle \delta | \hat{a}(k) | \gamma \rangle \tag{51}$$

with $\gamma \equiv |k_1 \dots k_N\rangle$ and $\delta \equiv |k'_1 \dots k'_{N-1}\rangle$, the operation of the annihilation operator for **fermions** turns out to be:

$$\hat{a}(k)|0\rangle = 0 \tag{52a}$$

$$\hat{a}(k)|k_1 \dots k_N\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (-1)^{i-1}\, \delta(k, k_i)|k_1 \dots k_{i-1}k_{i+1} \dots k_N\rangle \tag{52b}$$

To derive formula (52b) is a rather elaborate exercise, which is sketched below. Note that compared to (18b) for bosons we have an extra factor of $(-1)^{i-1}$ in (52b).

Derivation of (52b): Starting from (51) we consider:

$$\begin{aligned}
\langle k_1 \dots k_N|\hat{a}^\dagger(k)|k'_1 \dots k'_{N-1}\rangle &= \sqrt{N}\langle k_1 \dots k_N|kk'_1 \dots k'_{N-1}\rangle \\
&= \frac{\sqrt{N}}{N!} \sum_P \mathrm{sign}(P)\delta(k_{P1}, k)\delta(k_{P2}, k'_1) \dots \delta(k_{PN}, k'_{N-1}) \\
&= \frac{\sqrt{N}}{N!}\delta(k_1, k) \sum_{P'} \mathrm{sign}(P')\delta(k_{P'2}, k'_1) \dots \delta(k_{P'N}, k'_{N-1}) \\
+ \frac{\sqrt{N}}{N!}(-\delta(k_2, k)) \sum_{P''} &\mathrm{sign}(P'')\delta(k_{P''1}, k'_1)\delta(k_{P''3}, k'_2) \dots \delta(k_{P''N}, k'_{N-1}) \\
+ \quad \text{etc.},
\end{aligned}$$

where in the first step we used the definition of $\hat{a}^\dagger(k)$, in the second step formula (47); in the third step, we have split the sum over permutations P into N sums over permutations that leave 1 invariant ($P1 = 1$), take it to 2 ($P1 = 2$), etc. Since in the second term of the last step 1 and 2 have been interchanged we get an extra minus sign (we have taken: $P = P''P_{12}$, where P_{12} interchanges 1 and 2). Using (47) it is now easy to see that the sum over P' above can be written as:

$$\sum_{P'} \mathrm{sign}(P')\delta(k_{P'2}, k'_1) \dots \delta(k_{P'N}, k'_{N-1}) = (N-1)!\langle k_2 \dots k_N|k'_1 \dots k'_{N-1}\rangle \ ,$$

and the sum over P'' as:

$$\sum_{P''} \mathrm{sign}(P'')\delta(k_{P''1}, k'_1)\delta(k_{P''3}, k'_2) \dots \delta(k_{P''N}, k'_{N-1}) = (N-1)!\langle k_1 k_3 \dots k_N|k'_1 \dots k'_{N-1}\rangle \ ,$$

and similarly for the other sums over permutations. Now we can sum the terms again to:

$$\frac{1}{\sqrt{N}} \sum_{i=1}^{N} (-1)^{i-1}\, \delta(k_i, k)\langle k_1 \dots k_{i-1}k_{i+1} \dots k_N|k'_1 \dots k'_{N-1}\rangle$$

Taking the complex conjugate of this expression should, according to (51), equal: $\langle k'_1 \dots k'_{N-1}|\hat{a}(k)|k_1 \dots k_N\rangle$, so that (52b) can be read off.

c. Anti-commutation relations

From the definition of $\hat{a}^\dagger(k)$ and the derived result for $\hat{a}(k)$ it follows:

$$\left\{\hat{a}^\dagger(k), \hat{a}^\dagger(\ell)\right\} = \hat{0} \tag{53a}$$

$$\{\hat{a}(k), \hat{a}(\ell)\} = \hat{0} \tag{53b}$$

$$\left\{\hat{a}(k), \hat{a}^\dagger(\ell)\right\} = \delta(k,\ell)\,\hat{1} \tag{53c}$$

where $\left\{\hat{A}, \hat{B}\right\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ is the **anti-commutator** of two operators $\hat{A}$ and $\hat{B}$. Note that $\left\{\hat{A}, \hat{B}\right\} = \left\{\hat{B}, \hat{A}\right\}$.

Proof of (53c): First:

$$\hat{a}(k)\,\hat{a}^\dagger(\ell)|k_1 \ldots k_N\rangle = \hat{a}(k)\,\sqrt{N+1}|\ell\ k_1 \ldots k_N\rangle =$$

$$\frac{\sqrt{N+1}}{\sqrt{N+1}}\left[\delta(k,\ell)\,|k_1 \ldots k_N\rangle + \sum_{i=1}^{N}(-1)^i\,\delta(k,k_i)|\ell\ k_1 \ldots k_{i-1}k_{i+1} \ldots k_N\rangle\right] ,$$

where in the first step we have used (50b) and in the second step (52b), taking into account that the "ℓ-term" is the first term and the k_1-term is the second term, which therefore gets an extra minus-sign. Now we change the order of the operators and use (52b) first and (50b) second:

$$\hat{a}^\dagger(\ell)\,\hat{a}(k)|k_1 \ldots k_N\rangle = \hat{a}^\dagger(\ell)\,\frac{1}{\sqrt{N}}\sum_{i=1}^{N}(-1)^{i-1}\,\delta(k,k_i)|k_1 \ldots k_{i-1}k_{i+1} \ldots k_N\rangle =$$

$$\frac{\sqrt{N}}{\sqrt{N}}(-)\sum_{i=1}^{N}(-1)^i\,\delta(k,k_i)|\ell\ k_1 \ldots k_{i-1}k_{i+1} \ldots k_N\rangle$$

Adding the two results gives:

$$\left\{\hat{a}(k), \hat{a}^\dagger(\ell)\right\}|k_1 \ldots k_N\rangle = \delta(k,\ell)|k_1 \ldots k_N\rangle$$

Since the last result is for an arbitrary state vector in $\mathcal{E}$, we have shown (53c).

d. Many-body operators for fermions

This works analogously as for bosons: see formulae (25) and (26) for $\hat{F}$ and $\hat{G}$. It is important to note that for fermions (because of the anti-commutation relations) the order in which the creation- and annihilation operators appear is of significance.

e. Change of representation

This works exactly as for bosons: formulae (I.1) and (I.2).

7. Identical spin-$\frac{1}{2}$ particles

Application of the preceding: form of operators in *Second Quantization* for identical particles with mass m and spin $\frac{1}{2}$ (fermions!).

The one-fermion theory is often called "Schrödinger-Pauli theory". It's Hilbert space is again called $\mathcal{E}_1$.

Basis in discrete $\vec{k}$-representation in $\mathcal{E}_1$: $\left\{|\vec{k}\sigma\rangle\right\}$
$\vec{k} = \frac{2\pi}{L}\,\vec{n}$ with n_x, n_y, n_z integer numbers; $\sigma = +1$ or -1 (spin $\frac{1}{2}$).
In (continuous) $\vec{r}$-representation: $\{|\vec{r}\sigma\rangle\}$

The connection between the $\vec{k}\sigma$- and $\vec{r}\sigma$-representations is (cf. (I.8)):

$$\langle\vec{r}\sigma\,|\vec{k}\sigma'\rangle = \frac{1}{\sqrt{V}}\,e^{i\vec{k}\cdot\vec{r}}\,\delta_{\sigma,\sigma'} \tag{54}$$

a. The $\vec{k}\sigma$-representation

The form of operators for many-fermion systems is derived quite analogously to that for the bosonic case; one has to drag along an extra spin index σ, compared to the spin 0 case.

<u>Many-body operators</u>

$$\hat{n}_{\vec{k}\sigma} = \hat{a}^\dagger_{\vec{k}\sigma}\,\hat{a}_{\vec{k}\sigma} \tag{55}$$

$$\hat{n}_{\vec{k}} = \sum_\sigma \hat{n}_{\vec{k}\sigma} \tag{56}$$

$$\hat{N} = \sum_{\vec{k}\sigma} \hat{n}_{\vec{k}\sigma} \qquad \textbf{total particle number} \tag{57}$$

$$\hat{H^{(0)}} = \sum_{\vec{k}\sigma} \varepsilon_k \hat{n}_{\vec{k}\sigma} = \sum_{\vec{k}\sigma} \varepsilon_k\,\hat{a}^\dagger_{\vec{k}\sigma}\,\hat{a}_{\vec{k}\sigma} \qquad \text{with} \quad \varepsilon_k = \frac{\hbar^2 k^2}{2m} \tag{58}$$

We need to use our knowledge of the Hilbert space for spin-$\frac{1}{2}$ objects to find many-body operators that involve spin in a less trivial manner.

General procedure [cf. (27)-(28)]: (i) determine matrix elements

$$f_{\vec{k}\sigma,\vec{k}'\sigma'} = \langle\vec{k}\sigma|\hat{f}^{(1)}|\vec{k}'\sigma'\rangle \tag{59}$$

(ii) Using (i):

$$\hat{F} = \sum_{\vec{k}\sigma}\sum_{\vec{k}'\sigma'} \hat{a}^\dagger_{\vec{k}\sigma} f_{\vec{k}\sigma,\vec{k}'\sigma'} \hat{a}_{\vec{k}'\sigma'} \tag{60}$$

For instance, the operator $\hat{\Sigma}_x$, x-component of spin of the many-fermion system (in units of $\hbar/2$), is derived from the (one-particle) operator $\hat{\sigma}_x$ as follows (using the appropriate Pauli matrix):

$$\langle\vec{k}\sigma|\hat{\sigma}_x|\vec{k}'\sigma'\rangle = \delta_{\vec{k},\vec{k}'}\,[\delta_{\sigma,1}\,\delta_{\sigma',-1} + \delta_{\sigma,-1}\,\delta_{\sigma',1}] \qquad \longrightarrow$$

$$\hat{\Sigma}_x = \sum_{\vec{k}} \left[\hat{a}^\dagger_{\vec{k},1}\, \hat{a}_{\vec{k},-1} + \hat{a}^\dagger_{\vec{k},-1}\, \hat{a}_{\vec{k},1} \right] \tag{61a}$$

The other components of spin are (check for yourself):

$$\hat{\Sigma}_y = \sum_{\vec{k}} \left[-i\, \hat{a}^\dagger_{\vec{k},1}\, \hat{a}_{\vec{k},-1} + i\, \hat{a}^\dagger_{\vec{k},-1}\, \hat{a}_{\vec{k},1} \right] \tag{61b}$$

$$\hat{\Sigma}_z = \sum_{\vec{k}} \left[\hat{a}^\dagger_{\vec{k},1}\, \hat{a}_{\vec{k},1} - \hat{a}^\dagger_{\vec{k},-1}\, \hat{a}_{\vec{k},-1} \right] = \sum_{\vec{k}} \left(\hat{n}_{\vec{k},1} - \hat{n}_{\vec{k},-1} \right) \tag{61c}$$

It is important to note that not <u>all</u> commutators have to be replaced by anti-commutators in going from bosons to fermions. For instance, the dynamics of operators (Heisenberg picture) is still governed by the Heisenberg equations and these contain commutators. As an example we compute the time-dependence of the annihilation operator (in the $\vec{k}\sigma$-representation):

$$\frac{d}{dt}\left(\hat{a}_{\vec{k}\sigma}(t) \right) = \frac{i}{\hbar} \left[\hat{H}^{(0)}, \hat{a}_{\vec{k}\sigma}(t) \right] = \frac{i}{\hbar} \sum_{\vec{k}'\sigma'} \varepsilon_{k'} \left[\hat{a}^\dagger_{\vec{k}'\sigma'}\, \hat{a}_{\vec{k}'\sigma'}, \hat{a}_{\vec{k}\sigma} \right](t) \tag{62}$$

To compute the commutator we use the general operator formula:

$$\left[\hat{A}\hat{B}, \hat{C} \right] = \hat{A} \left\{ \hat{B}, \hat{C} \right\} - \left\{ \hat{A}, \hat{C} \right\} \hat{B} \tag{63}$$

(which is easily proved by writing out the (anti-)commutators). Using the anti-commutation relations we then find:

$$\left[\hat{a}^\dagger_{\vec{k}'\sigma'}\, \hat{a}_{\vec{k}'\sigma'}, \hat{a}_{\vec{k}\sigma} \right] = \hat{a}^\dagger_{\vec{k}'\sigma'} \cdot 0 \; - \; \delta_{\vec{k},\vec{k}'}\, \delta_{\sigma,\sigma'}\, \hat{a}_{\vec{k}'\sigma'}$$

Substituting in (62), we have:

$$\frac{d}{dt}\left(\hat{a}_{\vec{k}\sigma}(t) \right) = -\frac{i\varepsilon_k}{\hbar}\, \hat{a}_{\vec{k}\sigma}(t) \quad \longrightarrow \quad \hat{a}_{\vec{k}\sigma}(t) = \hat{a}_{\vec{k}\sigma}\, e^{-i\omega_k t} \;, \tag{64}$$

where $\omega_k = \varepsilon_k/\hbar$. Note that this is the same result as for bosons in (40), but that the calculation is quite different!

b. The $\vec{r}\sigma$-representation

The change of representation is now easily made using formulae (I.2) and (54):

$$\hat{a}_{\vec{k}\sigma} \qquad \longrightarrow \qquad \hat{\psi}(\vec{r}\sigma)$$

Mostly it is just a matter of replacing $\int d\vec{r} \ldots$ by $\sum_\sigma \int d\vec{r} \ldots$, but for spin operators there are some differences.

Examples

$$\hat{n}(\vec{r}\sigma) = \hat{\psi}^\dagger(\vec{r}\sigma)\,\hat{\psi}(\vec{r}\sigma) \tag{65}$$

$$\hat{n}(\vec{r}) = \sum_\sigma \hat{n}(\vec{r}\sigma) \tag{66}$$

$$\hat{N} = \sum_\sigma \int d\vec{r}\;\hat{n}(\vec{r}\sigma) \tag{67}$$

$$\hat{\Sigma}_x = \int d\vec{r}\left(\hat{\psi}^\dagger(\vec{r},1)\,\hat{\psi}(\vec{r},-1) + \hat{\psi}^\dagger(\vec{r},-1)\,\hat{\psi}(\vec{r},1)\right) \tag{68}$$

where the latter formula is an example of an operator which is non-diagonal in spin space. The above examples can all be obtained from the $\vec{k}\sigma$-representation forms by using the change-of-representation formula (cf. (34) for bosons):

$$\hat{\psi}(\vec{r}\sigma) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\,\hat{a}_{\vec{k}\sigma} \tag{69}$$

One could again view the many-fermion formalism as a "quantization" of the Schrödinger-Pauli wavefunction;

$$\psi(\vec{r}\sigma,t) \qquad \longrightarrow \qquad \hat{\psi}(\vec{r}\sigma,t)$$

("second quantization").

In summary, the second quantization formalism allows to express many-body operators for systems of identical, interacting particles with fluctuating particle number in terms of creation- and annihilation operators, which obey commutation relations (20) for bosons and anti-commutation relations (53) for fermions.

8. Bose-Einstein and Fermi-Dirac distributions

After the hard work of introducing the second quantization formalism and the experience with operator calculus in the earlier part of the course, it is now relatively easy to derive the important Bose-Einstein- and Fermi-Dirac distributions of quantum statistical physics.

$$\langle n_k\rangle = \frac{1}{e^{\beta(\varepsilon_k-\mu)}-1} \qquad \text{BE distribution} \tag{70}$$

$$\langle n_k\rangle = \frac{1}{e^{\beta(\varepsilon_k-\mu)}+1} \qquad \text{FD distribution} \quad , \tag{71}$$

where $\beta = 1/k_\mathrm{B}T$, k_B: Boltzmann's constant, T: absolute temperature, μ: chemical potential (= energy of adding a particle to the system: $\mu = \frac{\partial F}{\partial N}$, F: (Helmholtz) free energy).

Generally we have for an expectation value:

$$\langle A\rangle = \mathrm{Tr}\,(\hat{\rho}\,\hat{A}) \;, \tag{72}$$

where the trace Tr is taken in Fock space and the (grand-canonical) state operator (or: density operator) is given by:

$$\hat{\rho} = \frac{e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}}{\mathrm{Tr}\, e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}} = \frac{1}{\Xi}\, e^{-\beta\left(\hat{H}-\mu\hat{N}\right)} \tag{73}$$

$\hat{H}$ and $\hat{N}$ are taken as given in previous sections: $\hat{H}^{(0)}$ and $\hat{N}$. Ξ is the grand-canonical partition function. Our derivation will therefore be for free particles, but the results also hold for interacting particles if we can somehow define one-particle energies ε_k and occupation numbers n_k.

$$\langle n_k \rangle = \mathrm{Tr}\,(\hat{\rho}\,\hat{n}_k) = \frac{1}{\Xi}\,\mathrm{Tr}\,\left(e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\,\hat{a}_k^\dagger\,\hat{a}_k\right) \tag{74}$$

To compute the trace we need an operator identity that was derived in Exercise 2.4.11 in Le Bellac (see Problem Session 1):

$$e^{t\hat{A}}\,\hat{B}\,e^{-t\hat{A}} = \hat{B} + t\,\left[\hat{A},\hat{B}\right] + \frac{t^2}{2!}\,\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] + \cdots$$

For the special case that: $\left[\hat{A},\hat{B}\right] = \gamma\,\hat{B}$, we have (put $t = 1$):

$$e^{\hat{A}}\,\hat{B}\,e^{-\hat{A}} = e^{\gamma}\,\hat{B} \tag{75}$$

We furthermore need the following commutator, which holds for both bosons and fermions (!), as we calculated in previous sections:

$$\left[\hat{n}_k, \hat{a}_k^\dagger\right] = \hat{a}_k^\dagger \tag{76}$$

Then:

$$\left[\hat{H}-\mu\hat{N}, \hat{a}_k^\dagger\right] = (\varepsilon_k - \mu)\,\hat{a}_k^\dagger \longrightarrow e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\,\hat{a}_k^\dagger\,e^{\beta\left(\hat{H}-\mu\hat{N}\right)}\,e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\,\hat{a}_k = e^{-\beta(\varepsilon_k-\mu)}\,\hat{a}_k^\dagger\,e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\,\hat{a}_k\ ,$$

where we have used (75) in the last step (in the first step, convince yourself that the equality sign also holds for fermions!). From (74) it then follows;

$$\langle n_k \rangle = \frac{1}{\Xi}\,e^{-\beta(\varepsilon_k-\mu)}\,\mathrm{Tr}\,\left(\hat{a}_k^\dagger\,e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\hat{a}_k\right) = e^{-\beta(\varepsilon_k-\mu)}\,\langle \hat{a}_k\,\hat{a}_k^\dagger \rangle\ , \tag{77}$$

where in the first step we have used the previous formula and in the last step we performed a rotation of operators in the trace (which leaves it unchanged). Now the expectation value in formula (77) equals $\langle n_k \rangle + 1$ for **bosons** (commutation relation (20c)) and equals $-\langle n_k \rangle + 1$ for **fermions** (anti-commutation relation (53c)). Inserting this back into (77) one readily recovers the BE- and FD-distributions (70) and (71), respectively.