



Classic Fields

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CLASSICAL FIELDS

PARTICLES AND FIELDS

1. Variable number of particles
2. Interactions of different fields

Particles	Fields
$q_i(t)$	$\psi(\mathbf{r}, t)$ — field amplitudes
$\dot{q}_i(t)$	$\dot{\psi}(\mathbf{r}, t)$
$L(q, \dot{q})$	$L[\psi, \nabla\psi, \dot{\psi}] = \int_V \mathcal{L}(\psi, \nabla\psi, \dot{\psi}) d^3x$
$p_i = \frac{\partial L}{\partial \dot{q}_i}$	$\pi(\mathbf{r}, t) = \frac{\partial \mathcal{L}}{\partial \dot{\psi}}$ — momentum density
$H(p, q)$	$H[\psi, \nabla\psi, \pi, \nabla\pi] = \int_V \mathcal{H}(\psi, \nabla\psi, \pi, \nabla\pi) d^3x$

\mathcal{L} – Lagrangian density; \mathcal{H} – Hamiltonian density

PRINCIPLE OF THE LEAST ACTION

Particles	Fields
$\delta \int_{t_1}^{t_2} L(q, \dot{q}) dt = 0$ $\delta q_i(t_1) = \delta q_i(t_2) = 0$	$\delta \int_{t_1}^{t_2} L[\psi, \nabla\psi, \dot{\psi}] dt = 0$ $\delta \psi(\mathbf{r}, t_1) = \delta \psi(\mathbf{r}, t_2) = 0$

$$\delta \int_{t_1}^{t_2} L[\psi, \nabla\psi, \dot{\psi}] dt = \int_{t_1}^{t_2} \int_V \delta \mathcal{L}(\psi, \nabla\psi, \dot{\psi}) d^3x dt = 0$$

$$\delta \mathcal{L} = \frac{\partial \mathcal{L}}{\partial \psi} \delta \psi + \frac{\partial \mathcal{L}}{\partial \nabla \psi} \delta(\nabla \psi) + \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \delta \dot{\psi}$$

$$\delta \dot{\psi} = \frac{\partial}{\partial t}(\delta \psi), \quad \delta(\nabla \psi) = \nabla(\delta \psi)$$

EULER-LAGRANGE EQUATIONS

Integration by parts, } \Rightarrow
 Condition that ψ and $\delta\psi$ vanish on $S(V)$,

$$\int_{t_1}^{t_2} \int_V \left[\frac{\partial \mathcal{L}}{\partial \psi} - \nabla \left(\frac{\partial \mathcal{L}}{\partial (\nabla \psi)} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{\psi}} \right) \right] \delta\psi d^3x dt = 0$$

$$\frac{\partial \mathcal{L}}{\partial \psi} - \nabla \left(\frac{\partial \mathcal{L}}{\partial (\nabla \psi)} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{\psi}} \right) = 0,$$

where $S(V)$ is the surface surrounding V . If $x_\mu = (\mathbf{r}, ict)$ then

$$\frac{\partial \mathcal{L}}{\partial \psi} - \frac{\partial}{\partial x_\mu} \left(\frac{\partial \mathcal{L}}{\partial \psi_{,\mu}} \right) = 0.$$

The equation is covariant if \mathcal{L} is invariant under Lorentz transformation.

THE HAMILTONIAN

Particles	Fields
$H(q, p) = \sum_i p_i \dot{q}_i - L$	$\mathcal{H}(\psi, \nabla\psi, \pi, \nabla\pi) = \pi\dot{\psi} - \mathcal{L}$

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}}, \quad H = \int_V \mathcal{H} d^3x.$$

$$\begin{aligned} \int_V \delta \mathcal{L} d^3x &= \int_V \left\{ \left[\frac{\partial \mathcal{L}}{\partial \psi} - \nabla \cdot \left(\frac{\partial \mathcal{L}}{\partial (\nabla \psi)} \right) \right] \delta \psi + \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \delta \dot{\psi} \right\} d^3x \\ &= \int_V \left(\dot{\pi} \delta \psi + \pi \delta \dot{\psi} \right) d^3x \\ &= \int_V \left[\delta(\pi \dot{\psi}) - \dot{\psi} \delta \pi + \dot{\pi} \delta \psi \right] d^3x \\ &= \int_V \left[\delta(\mathcal{H} + \mathcal{L}) - \dot{\psi} \delta \pi + \dot{\pi} \delta \psi \right] d^3x. \end{aligned}$$

THE HAMILTON EQUATIONS

$$\int_V \delta \mathcal{H} d^3 x = \int_V \left(\dot{\psi} \delta \pi - \dot{\pi} \delta \psi \right) d^3 x$$

$$\begin{aligned} \delta H &= \delta \int_V \mathcal{H} d^3 x = \int_V \left(\dot{\psi} \delta \pi - \dot{\pi} \delta \psi \right) d^3 x \\ &= \int_V \left\{ \frac{\partial \mathcal{H}}{\partial \pi} \delta \pi + \frac{\partial \mathcal{H}}{\partial \nabla \pi} \delta(\nabla \pi) + \frac{\partial \mathcal{H}}{\partial \psi} \delta \psi + \frac{\partial \mathcal{H}}{\partial \nabla \psi} \delta(\nabla \psi) \right\} d^3 x \\ &= \int_V \left\{ \left[\frac{\partial \mathcal{H}}{\partial \pi} - \nabla \frac{\partial \mathcal{H}}{\partial \nabla \pi} \right] \delta \pi + \left[\frac{\partial \mathcal{H}}{\partial \psi} - \nabla \frac{\partial \mathcal{H}}{\partial \nabla \psi} \right] \delta \psi \right\} d^3 x \end{aligned}$$

$$\begin{aligned} \dot{\psi} &= \frac{\partial \mathcal{H}}{\partial \pi} - \nabla \frac{\partial \mathcal{H}}{\partial \nabla \pi} \\ -\dot{\pi} &= \frac{\partial \mathcal{H}}{\partial \psi} - \nabla \frac{\partial \mathcal{H}}{\partial \nabla \psi} \end{aligned}$$

SOME PROPERTIES OF THE LAGRANGIAN DENSITY

- The equation of motion derived from the Lagrangian densities \mathcal{L} and

$$\mathcal{L}' = a (\mathcal{L} + F_{\mu,\mu}) = a \left(\mathcal{L} + \nabla \mathbf{F} + \frac{\partial F_4}{\partial t} \right),$$

where a is a constant and F_{μ} vanishes at $S(V)$, are the same.

- The Lagrangian density must behave as a scalar.
- If the order of the equation of motion has to be at most 2, the Lagrangian density may only depend on ψ and $\psi_{,\mu}$
- The Lagrangian density has to be real (Hermitian in quantized theories)

EXAMPLES

A real scalar field

$$\mathcal{L}(\psi, \psi_{,\mu}) = -\frac{1}{2} (\psi_{,\mu}\psi_{,\mu} + \kappa^2\psi^2)$$

The resulting Euler-Lagrange equation:

$$\left(\frac{\partial^2}{\partial x_\mu^2} - \kappa^2 \right) \psi = 0, \quad \text{i.e.} \quad (\square - \kappa^2)\psi = 0,$$

where $\square = \frac{\partial^2}{\partial x_\mu^2} = \Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}$ – d'Alembert operator.

If

$$E^2 = p^2 c^2 + m^2 c^4$$
$$E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad \mathbf{p} \rightarrow -i\hbar \nabla$$

then $\kappa = \frac{mc}{\hbar}$ and we get the Klein-Gordon equation.

Yukawa potential

Interaction: $\mathcal{L}_{\text{int}} = -\psi\rho$

$$(\square - \kappa^2)\psi = \rho, \quad \text{let } \rho = G\delta(\mathbf{r})$$

In the case of a static (time-independent) field:

$$(\Delta - \kappa^2)\psi = G\delta(\mathbf{r})$$

Let us define $\tilde{\psi}(\mathbf{k})$ as

$$\tilde{\psi}(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int_V e^{-i\mathbf{k}\cdot\mathbf{r}} \psi(\mathbf{r}) d^3x, \quad \text{i.e.}$$

$$\psi(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int_{V_k} e^{i\mathbf{k}\cdot\mathbf{r}} \tilde{\psi}(\mathbf{k}) d^3k, \quad \text{i.e.}$$

Then

$$-(k^2 + \kappa^2) \tilde{\psi}(\mathbf{k}) = \frac{G}{(2\pi)^{3/2}}$$

$$\tilde{\psi}(\mathbf{k}) = -\frac{1}{(2\pi)^{3/2}} \frac{G}{k^2 + \kappa^2}$$

and

$$\psi(\mathbf{r}) = -\frac{G}{4\pi} \frac{e^{-\kappa r}}{r}$$

$$\psi(\mathbf{r}_2) = -\frac{G}{4\pi} \frac{e^{-\kappa |\mathbf{r}_2 - \mathbf{r}_1|}}{|\mathbf{r}_2 - \mathbf{r}_1|}$$

$$\mathcal{H}_{\text{int}} = -\mathcal{L}_{\text{int}} = \psi\rho = -\frac{G}{4\pi} \frac{e^{-\kappa |\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} G\delta(\mathbf{r}')$$

$$H_{\text{int}} = \int_V \mathcal{H}_{\text{int}} d^3x' = -\frac{G^2}{4\pi} \frac{e^{-\kappa r}}{r}$$

A complex scalar field

The field amplitude has two-components: ψ, ψ^* .

Two component real field:

$$\begin{aligned}\psi_1 &= \frac{1}{\sqrt{2}} (\psi + \psi^*) \\ \psi_2 &= \frac{1}{i\sqrt{2}} (\psi - \psi^*)\end{aligned}$$

$$\begin{aligned}\mathcal{L} &= -\frac{1}{2} \sum_{s=1}^2 \left[\left(\frac{\partial \psi_s}{\partial x_\mu} \right)^2 + \kappa^2 \psi_s^2 \right] \\ &= -\psi_{,\mu}^* \psi_{,\mu} - \kappa^2 \psi^* \psi.\end{aligned}$$

$$\text{From here: } \begin{cases} (\square - \kappa^2) \psi^* = 0 \\ (\square - \kappa^2) \psi = 0 \end{cases}$$

In an external field

$$-i\hbar \frac{\partial}{\partial x_\mu} \rightarrow -i\hbar \frac{\partial}{\partial x_\mu} - \frac{e}{c} A_\mu$$

If ψ corresponds to $A_\mu = (0, 0, 0, iA_0)$
then ψ^* corresponds to $A_\mu = (0, 0, 0, -iA_0)$.

Consequently,

$$\begin{aligned} \psi &\leftrightarrow \psi^* \\ e &\leftrightarrow -e \end{aligned}$$

Four-vector current in the complex field

$$\begin{array}{l} \psi'_1 = \psi_1 \cos \lambda - \psi_2 \sin \lambda \\ \psi'_2 = \psi_1 \sin \lambda + \psi_2 \cos \lambda \end{array} \left\| \begin{array}{l} \psi' = e^{i\lambda} \psi \\ \psi^{*'} = e^{-i\lambda} \psi^* \end{array} \right.$$

For infinitesimal λ :

$$\delta\psi = i\lambda\psi, \quad \delta\psi^* = -i\lambda\psi^*$$

$$\delta = -i\lambda \frac{\partial}{\partial x_\mu} \left(\frac{\partial\psi^*}{\partial x_\mu} \psi - \psi^* \frac{\partial\psi}{\partial x_\mu} \right), \text{ i.e.}$$

$$\frac{\partial j_\mu}{\partial x_\mu} = 0 \text{ with } j_\mu = i \left(\frac{\partial\psi^*}{\partial x_\mu} \psi - \psi^* \frac{\partial\psi}{\partial x_\mu} \right)$$

Again

$$\psi \leftrightarrow \psi^*$$

$$j_\mu \leftrightarrow -j_\mu$$

The Schrödinger field

$$\mathcal{L} = \frac{i\hbar}{2}(\psi^* \dot{\psi} - \dot{\psi}^* \psi) - \frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi - V(\mathbf{r}) \psi^* \psi$$

Let $\mathbf{F} \sim \nabla(\psi^* \psi)$, $F_4 \sim \psi^* \psi$. Then

$$\nabla \mathbf{F} \sim \Delta(\psi^* \psi) = 2\nabla \psi^* \nabla \psi + (\Delta \psi^*) \psi + \psi^* (\Delta \psi)$$

$$\frac{\partial F_4}{\partial t} \sim \psi^* \dot{\psi} + \dot{\psi}^* \psi$$

Therefore in the Lagrangian density one can replace

$$\frac{1}{2}(\psi^* \dot{\psi} - \dot{\psi}^* \psi) \quad \text{by} \quad \psi^* \dot{\psi}$$

Commonly used form of the Lagrangian density:

$$\mathcal{L} = i\hbar \psi^* \dot{\psi} - \frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi - V(\mathbf{r}) \psi^* \psi$$

Euler-Lagrange equations:

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi$$

$$-i\hbar\dot{\psi}^* = -\frac{\hbar^2}{2m}\Delta\psi^* + V\psi^*$$

Hamiltonian formalism:

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\hbar\psi^*, \quad \pi^* = 0$$

$$\begin{aligned} \mathcal{H} &= \sum_s \pi_s \dot{\psi}_s - \mathcal{L} = \pi \dot{\psi} + \psi^* \dot{\psi}^* - \mathcal{L} = i\hbar\psi^* \dot{\psi} - \mathcal{L} \\ &= \frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi + V(\mathbf{r}) \psi^* \psi \\ &= -\frac{i\hbar}{2m} \nabla \psi \nabla \pi - \frac{i}{\hbar} V(\mathbf{r}) \psi \pi \end{aligned}$$

$$\text{Hamilton equations: } \begin{cases} i\hbar\dot{\psi} = -\frac{\hbar^2}{2m} \Delta \psi + V \psi \\ -i\hbar\dot{\pi} = -\frac{\hbar^2}{2m} \Delta \pi + V \pi \end{cases}$$

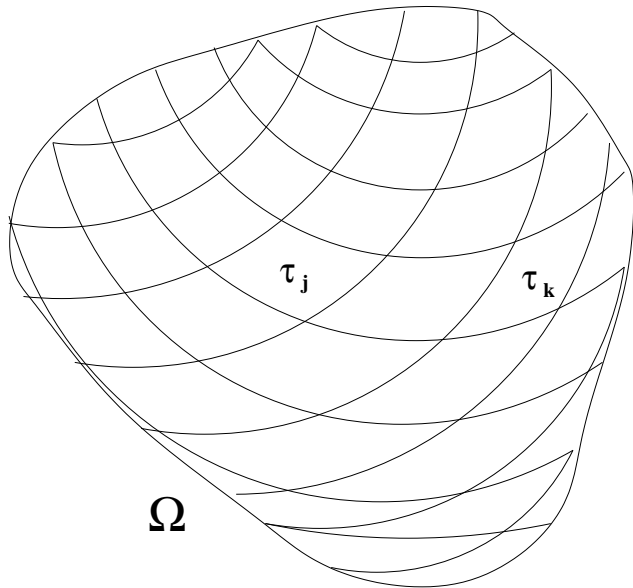
QUANTIZATION

Discretization of the field

We discretize the volume V by dividing it to cells. In each cell ψ and π may be assumed to be constant. Thus, in the j -th cell

$$\psi_j \equiv \psi(\mathbf{r}_j, t), \quad \pi_j \equiv \pi(\mathbf{r}_j, t), \quad P_j = \tau_j \pi_j,$$

τ_j, P_j – the volume and the momentum corresponding to the j -th cell.



	particles	fields
classical	q_j, p_j	ψ_j, P_j
quantum	\hat{q}_j, \hat{p}_j	$\hat{\psi}_j, \hat{P}_j$

Application of the correspondence principle

$$\begin{aligned} [\hat{q}_j, \hat{q}_k] &= [\hat{p}_j, \hat{p}_k] = 0, & [\hat{q}_j, \hat{p}_k] &= i\hbar\delta_{jk} \\ [\hat{\psi}_j, \hat{\psi}_k] &= [\hat{P}_j, \hat{P}_k] = 0, & [\hat{\psi}_j, \hat{P}_k] &= i\hbar\delta_{jk} \end{aligned}$$

$$\hat{\psi}_j \rightarrow \hat{\psi}(\mathbf{r}, t) \equiv \hat{\psi}; \quad \hat{\psi}_k \rightarrow \hat{\psi}(\mathbf{r}', t) \equiv \hat{\psi}'$$

$$[\hat{\psi}, \hat{\psi}'] = [\hat{\pi}, \hat{\pi}'] = 0 \quad \left[\hat{\psi}, \hat{\pi}' \right] = i\hbar \lim_{\tau_k \rightarrow 0} \frac{\delta_{jk}}{\tau_k} = i\hbar\delta(\mathbf{r} - \mathbf{r}')$$

But $\pi = i\hbar\psi^*$. Therefore $\hat{\pi} = i\hbar\hat{\psi}^\dagger$, and

$$\left[\hat{\psi}, \hat{\psi}' \right] = \left[\hat{\psi}^\dagger, \hat{\psi}'^\dagger \right] = 0, \quad \left[\hat{\psi}, \hat{\psi}'^\dagger \right] = \delta(\mathbf{r} - \mathbf{r}')$$

$\hat{\psi}$ – the field operator

Hamiltonian and the equations of motion

$$\mathcal{H} = \frac{\hbar^2}{2m} \nabla \psi^* \nabla \psi + V(\mathbf{r}) \psi^* \psi$$

$$\hat{\mathcal{H}} = \frac{\hbar^2}{2m} \nabla \hat{\psi}^\dagger \nabla \hat{\psi} + V(\mathbf{r}) \hat{\psi}^\dagger \hat{\psi}$$

$$\hat{H} = \int_V \hat{\mathcal{H}} d^3x = \int_V \hat{\psi}^\dagger \left(-\frac{\hbar^2}{2m} \Delta + V \right) \hat{\psi} d^3x$$

Note:
$$\int_V (\nabla \hat{\psi}^\dagger) (\nabla \hat{\psi}) d^3\mathbf{r} = - \int_V \hat{\psi}^\dagger \Delta \hat{\psi} d^3\mathbf{r} + \underbrace{\int_{S(V)} \hat{\psi}^\dagger \nabla \hat{\psi} d\boldsymbol{\sigma}}_{=0}$$

Heisenberg equation for $\hat{\psi}$:
$$i\hbar \dot{\hat{\psi}} = [\hat{\psi}, \hat{H}]$$

Finally, after the evaluation of the commutator:

$$i\hbar \dot{\hat{\psi}} = -\frac{\hbar^2}{2m} \Delta \hat{\psi} + V(\mathbf{r}) \hat{\psi}$$

The evaluation of $[\hat{\psi}, \hat{H}]$:

$$\begin{aligned} & \left[\hat{\psi}, \int_V \hat{\psi}'^\dagger V' \hat{\psi}' d^3 \mathbf{r}' \right] = \int_V \left(\hat{\psi} \hat{\psi}'^\dagger - \hat{\psi}'^\dagger \hat{\psi} \right) V' \hat{\psi}' d^3 \mathbf{r}' \\ & = \int_V \delta(\mathbf{r} - \mathbf{r}') V' \hat{\psi}' d^3 \mathbf{r}' = V \hat{\psi}, \end{aligned}$$

$$\begin{aligned} & \left[\hat{\psi}, \int_V \hat{\psi}'^\dagger \Delta' \hat{\psi}' d^3 \mathbf{r}' \right] = \int_V \left(\hat{\psi} \hat{\psi}'^\dagger - \hat{\psi}'^\dagger \hat{\psi} \right) \Delta' \hat{\psi}' d^3 \mathbf{r}' \\ & = \int_V \delta(\mathbf{r} - \mathbf{r}') \Delta' \hat{\psi}' d^3 \mathbf{r}' = \Delta \hat{\psi}, \end{aligned}$$

Constants of the motion

The set of the constants of the motion include the operator of the number of particles

$$\hat{N} = \int_V \hat{\psi}^\dagger \hat{\psi} d^3x$$

and the commutators

$$\left[\hat{\psi}, \hat{\psi}' \right], \quad \left[\hat{\psi}^\dagger, \hat{\psi}'^\dagger \right], \quad \left[\hat{\psi}, \hat{\psi}'^\dagger \right].$$

The demonstration that they commute with \hat{H} is straightforward and involves the evaluation of commutators of products of two field operators, as e.g.:

$$\begin{aligned} \left[\hat{\psi}^\dagger \hat{\psi}, \hat{\psi}'^\dagger \hat{\psi}' \right] &= \hat{\psi}^\dagger \hat{\psi} \hat{\psi}'^\dagger \hat{\psi}' - \hat{\psi}'^\dagger \hat{\psi}' \hat{\psi}^\dagger \hat{\psi} \\ &= \hat{\psi}^\dagger \hat{\psi}'^\dagger \hat{\psi} \hat{\psi}' - \hat{\psi}'^\dagger \hat{\psi}^\dagger \hat{\psi}' \hat{\psi} + \delta(\mathbf{r} - \mathbf{r}') \left(\hat{\psi}^\dagger \hat{\psi}' - \hat{\psi}'^\dagger \hat{\psi} \right) = 0 \end{aligned}$$

THE NUMBER REPRESENTATION

The number representation

In this representation the basis in the Hilbert space is formed by the eigenvectors of \hat{N} . Let $u_k(\mathbf{r})$, $k = 1, 2, \dots$ be a complete, discrete and orthonormal set of functions. Thus,

$$\int_V u_k^*(\mathbf{r})u_l(\mathbf{r})d^3x = \delta_{kl},$$

$$\hat{\psi}(\mathbf{r}, t) = \sum_k \hat{a}_k(t)u_k(\mathbf{r}) \quad \hat{\psi}(\mathbf{r}, t)^\dagger = \sum_k \hat{a}_k^\dagger(t)u_k^*(\mathbf{r}),$$

$$\hat{a}_k(t) = \int_V u_k^*(\mathbf{r})\hat{\psi}(\mathbf{r}, t)d^3x \quad \hat{a}_k^\dagger(t) = \int_V \hat{\psi}(\mathbf{r}, t)^\dagger u_k(\mathbf{r})d^3x$$

The commutation rules

$$\left[\hat{\psi}, \hat{\psi}' \right] = \left[\hat{\psi}^\dagger, \hat{\psi}'^\dagger \right] = 0, \quad \left[\hat{\psi}, \hat{\psi}'^\dagger \right] = \delta(\mathbf{r} - \mathbf{r}')$$

imply
$$\left[\hat{a}_k, \hat{a}_l \right] = \left[\hat{a}_k^\dagger, \hat{a}_l^\dagger \right] = 0, \quad \left[\hat{a}_k, \hat{a}_l^\dagger \right] = \delta_{kl}$$

The operator of the number of particles:

$$\begin{aligned}\hat{N} &= \int_V \hat{\psi}^\dagger \hat{\psi} d^3x = \sum_{kl} \hat{a}_k^\dagger \hat{a}_l \int_V u_k^* u_l d^3x \\ &= \sum_k \hat{a}_k^\dagger \hat{a}_k \equiv \sum_k \hat{N}_k\end{aligned}$$

The occupation number operator:

$$\hat{N}_k = \hat{a}_k^\dagger \hat{a}_k$$

It is easy to see that

$$[\hat{N}_k, \hat{N}_l] = 0.$$

In the number representation the set of commuting operators:

$$\hat{N}, \hat{N}_1, \hat{N}_2, \dots$$

is diagonal

Properties of $\hat{a}_k, \hat{a}_k^\dagger, \hat{N}_k$

Let us select a single value of k and denote, for the time being,

$$\hat{a} \equiv \hat{a}_k, \quad \hat{a}^\dagger \equiv \hat{a}_k^\dagger, \quad \hat{N} = \hat{a}^\dagger \hat{a} \equiv \hat{N}_k. \quad \text{Then,} \quad [\hat{a}, \hat{a}^\dagger] = 1$$

If $\hat{N}|n\rangle = n|n\rangle$, $|n'\rangle = \hat{a}|n\rangle$ then $\langle n|\hat{N}|n\rangle = \langle n|\hat{a}^\dagger \hat{a}|n\rangle = \langle n'|n'\rangle \geq 0$.

- $\hat{a}\hat{N} = \hat{a}\hat{a}^\dagger \hat{a} = (\hat{a}^\dagger \hat{a} + 1)\hat{a} = (\hat{N} + 1)\hat{a}$

$$\hat{a}\hat{N}|n\rangle = \begin{cases} (\hat{N} + 1)\hat{a}|n\rangle \\ n\hat{a}|n\rangle \end{cases} \Rightarrow \hat{N}(\hat{a}|n\rangle) = (n-1)(\hat{a}|n\rangle) \Rightarrow \hat{a}|n\rangle \sim |n-1\rangle$$

$$\hat{a}|1\rangle = |0\rangle, \quad \hat{a}|0\rangle = 0.$$

- $\hat{a}^\dagger \hat{N} = \hat{a}^\dagger \hat{a}^\dagger \hat{a} = (\hat{a}^\dagger \hat{a} - 1)\hat{a}^\dagger = (\hat{N} - 1)\hat{a}^\dagger$

$$\hat{a}^\dagger \hat{N}|n\rangle = \begin{cases} (\hat{N} - 1)\hat{a}^\dagger|n\rangle \\ n\hat{a}^\dagger|n\rangle \end{cases} \Rightarrow \hat{N}(\hat{a}^\dagger|n\rangle) = (n+1)(\hat{a}^\dagger|n\rangle) \Rightarrow \hat{a}^\dagger|n\rangle \sim |n+1\rangle$$

$$\begin{aligned}
\hat{a}^\dagger|0\rangle &= f(1)|1\rangle, \\
\hat{a}^\dagger|1\rangle &= f(2)|2\rangle = \frac{\hat{a}^\dagger\hat{a}^\dagger}{f(1)}|0\rangle, \\
&\dots \\
\hat{a}^\dagger|n-1\rangle &= f(n)|n\rangle = \frac{(\hat{a}^\dagger)^n}{f(1)f(2)\cdots f(n-1)}|0\rangle. \\
|n\rangle &= \frac{(\hat{a}^\dagger)^n}{f(1)f(2)\cdots f(n-1)f(n)}|0\rangle
\end{aligned}$$

One can show by induction that

$$\left[\hat{a}, (\hat{a}^\dagger)^n \right] = n (\hat{a}^\dagger)^{n-1}$$

This implies

$$\langle n|n\rangle = \frac{n!}{[f(1)f(2)\cdots f(n)]^2} = 1 \Rightarrow f(n) = \sqrt{n}.$$

$$\hat{a}^\dagger |n\rangle = f(n+1)|n+1\rangle \Rightarrow \hat{a}^\dagger |n\rangle = \sqrt{n+1}|n+1\rangle.$$

$$\hat{a}\hat{a}^\dagger |n-1\rangle = \sqrt{n}\hat{a}|n\rangle = (1 + \hat{N})|n-1\rangle = n|n-1\rangle; \Rightarrow \hat{a}|n\rangle = \sqrt{n}|n-1\rangle.$$

$$|0\rangle \leftrightarrow \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, |1\rangle \leftrightarrow \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}, |2\rangle \leftrightarrow \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{bmatrix}, \dots$$

$$\hat{a} \leftrightarrow \begin{pmatrix} 0 & \sqrt{1} & 0 & \dots & 0 & \dots \\ 0 & 0 & \sqrt{2} & \dots & 0 & \dots \\ 0 & 0 & 0 & \dots & 0 & \dots \\ \dots & & & & \dots & \\ 0 & 0 & 0 & \dots & \sqrt{n} & \dots \\ \dots & & & & \dots & \end{pmatrix} \hat{a}^\dagger \leftrightarrow \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & \dots \\ \sqrt{1} & 0 & 0 & \dots & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots & 0 & \dots \\ \dots & & & & \dots & \\ 0 & 0 & 0 & \dots & \sqrt{n} & \dots \\ \dots & & & & \dots & \end{pmatrix}$$

The general case: $\hat{N} = \sum_k \hat{N}_k$

The orthonormal basis of eigenvectors of \hat{N} , \hat{N}_1 , $\hat{N}_2, \dots, \hat{N}_k, \dots$:
 $|n_1, n_2, \dots, n_k, \dots\rangle$

$$\begin{aligned}\hat{N}_k |n_1, n_2, \dots, n_k, \dots\rangle &= n_k |n_1, n_2, \dots, n_k, \dots\rangle \\ \hat{a}_k |n_1, n_2, \dots, n_k, \dots\rangle &= \sqrt{n_k} |n_1, n_2, \dots, n_k - 1, \dots\rangle \\ \hat{a}_k^\dagger |n_1, n_2, \dots, n_k, \dots\rangle &= \sqrt{n_k + 1} |n_1, n_2, \dots, n_k + 1, \dots\rangle\end{aligned}$$

\hat{a}_k – annihilation operator
 \hat{a}_k^\dagger – creation operator

} of the k -th state of the field

The eigenvalue problem of the Hamiltonian

$$\hat{H} = \int_V \hat{\psi}^\dagger \left(-\frac{\hbar^2}{2m} \Delta + V \right) \hat{\psi} d^3x = \sum_{k,l} \hat{a}_k^\dagger \hat{a}_l h_{kl},$$

$$h_{kl} = \int_V u_k^* \left(-\frac{\hbar^2}{2m} \Delta + V \right) u_l d^3x$$

If $\left(-\frac{\hbar^2}{2m} \Delta + V \right) u_k = \mathcal{E}_k u_k$ then $h_{kl} = \mathcal{E}_k \delta_{kl}$,

$$\hat{H} = \sum_k \mathcal{E}_k \hat{a}_k^\dagger \hat{a}_k = \sum_k \mathcal{E}_k \hat{N}_k$$

$$i\hbar \dot{\hat{N}}_k = \left[\hat{a}_k^\dagger \hat{a}_k, \hat{H} \right] = 0,$$

and $\hat{H} |n_1, n_2, \dots, n_k, \dots\rangle = E |n_1, n_2, \dots, n_k, \dots\rangle,$

$$E = \sum_k n_k \mathcal{E}_k$$

Bosons and fermions

The formalism derived from the correspondence principle (the commutation rules for the field operators are the analogs of the commutation rules for the coordinate and momentum) describe bosons – the occupation numbers n_k may be arbitrary non-negative integers. For fermions $n_k = 0, 1$.

P. Jordan, E. Wigner, 1928 – in order to describe fermions, one has to replace commutators by anticommutators:

$$[\dots, \dots] \Rightarrow \{\dots, \dots\}$$

Bosons:

$$[\hat{\psi}, \hat{\psi}'] = [\hat{\psi}^\dagger, \hat{\psi}'^\dagger] = 0, \quad [\hat{\psi}, \hat{\psi}'^\dagger] = \delta(\mathbf{r} - \mathbf{r}')$$

Fermions:

$$\{\hat{\psi}, \hat{\psi}'\} = \{\hat{\psi}^\dagger, \hat{\psi}'^\dagger\} = 0, \quad \{\hat{\psi}, \hat{\psi}'^\dagger\} = \delta(\mathbf{r} - \mathbf{r}')$$

Fermions:

$$\begin{aligned}\{\hat{a}_k, \hat{a}_l\} = 0 &\Rightarrow \hat{a}_k \hat{a}_l = -\hat{a}_l \hat{a}_k \Rightarrow \hat{a}_k^2 = 0 \\ \{\hat{a}_k^\dagger, \hat{a}_l^\dagger\} = 0 &\Rightarrow \hat{a}_k^\dagger \hat{a}_l^\dagger = -\hat{a}_l^\dagger \hat{a}_k^\dagger \Rightarrow \hat{a}_k^{\dagger 2} = 0 \\ \{\hat{a}_k, \hat{a}_l^\dagger\} &= \delta_{kl}\end{aligned}$$

$$\hat{N}_k = \hat{a}_k^\dagger \hat{a}_k \Rightarrow \hat{N}_k^2 = \hat{a}_k^\dagger \hat{a}_k \hat{a}_k^\dagger \hat{a}_k = \hat{a}_k^\dagger (1 - \hat{a}_k^\dagger \hat{a}_k) \hat{a}_k = \hat{N}_k$$

Then,

$$\hat{N}_k (\hat{N}_k - 1) = 0 \Rightarrow n_k (n_k - 1) = 0 \Rightarrow n_k = 0, 1.$$

The remaining part of the formalism is the same. In particular:

$$\begin{aligned}i\hbar\hat{\psi} = [\hat{\psi}, \hat{H}] &= -\frac{\hbar^2}{2m}\Delta\hat{\psi} + V(\mathbf{r})\hat{\psi} \\ [\hat{N}_k, \hat{N}_l] = 0, \quad \hat{N} = 0, \quad E &= \sum_k n_k \mathcal{E}_k\end{aligned}$$

Properties of fermionic operators $\hat{a}_k, \hat{a}_k^\dagger, \hat{N}_k$

Let us denote $\hat{a} \equiv \hat{a}_k, \hat{a}^\dagger \equiv \hat{a}_k^\dagger, \hat{N} = \hat{a}^\dagger \hat{a} \equiv \hat{N}_k$.

Then, $\hat{a}^2 = \hat{a}^{\dagger 2} = 0, \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 1$.

$$\left. \begin{array}{l} \hat{a}|0\rangle = 0 \\ \hat{a}|1\rangle = |0\rangle \end{array} \right\} \Rightarrow \hat{a}|n\rangle = n|1-n\rangle$$

$$\left. \begin{array}{l} \hat{a}^\dagger|0\rangle = |1\rangle \\ \hat{a}^\dagger|1\rangle = 0 \end{array} \right\} \Rightarrow \hat{a}^\dagger|n\rangle = (1-n)|1-n\rangle$$

$$|0\rangle \leftrightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle \leftrightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

$$\hat{a} \leftrightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{a}^\dagger \leftrightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \hat{N} = \hat{a}^\dagger \hat{a} \leftrightarrow \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

The general case: $\hat{N} = \sum_k \hat{N}_k$

The orthonormal basis of eigenvectors of \hat{N} , \hat{N}_1 , $\hat{N}_2, \dots, \hat{N}_k, \dots$:

$|n_1, n_2, \dots, n_k, \dots\rangle$

$$\begin{aligned} \hat{N}_k |n_1, n_2, \dots, n_k, \dots\rangle &= n_k |n_1, n_2, \dots, n_k, \dots\rangle \\ \hat{a}_k |n_1, n_2, \dots, n_k, \dots\rangle &= \Theta_k n_k |n_1, n_2, \dots, 1 - n_k, \dots\rangle \\ \hat{a}_k^\dagger |n_1, n_2, \dots, n_k, \dots\rangle &= \Theta_k (1 - n_k) |n_1, n_2, \dots, 1 - n_k, \dots\rangle \end{aligned}$$

$$\Theta_k = (-1)^{\nu_k}, \quad \nu_k = \sum_{j=1}^{k-1} n_j$$

The phase factors Θ_k are introduced in order to secure that

$$\hat{a}_k \hat{a}_l |n_1, n_2, \dots, n_k, \dots\rangle = -\hat{a}_l \hat{a}_k |n_1, n_2, \dots, n_k, \dots\rangle$$

MAXWELL FIELD

MAXWELL EQUATIONS

$$\left. \begin{aligned} \nabla \mathbf{E} &= \frac{\rho}{\epsilon_0}, \\ \nabla \times \mathbf{B} - \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} &= \mu_0 \mathbf{j} \end{aligned} \right\} \frac{1}{\mu_0} \frac{\partial F_{\mu\nu}}{\partial x_\nu} = j_\mu$$

$$\left. \begin{aligned} \nabla \mathbf{B} &= 0, \\ \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} &= 0 \end{aligned} \right\} \frac{\partial F_{\mu\nu}}{\partial x_\lambda} + \frac{\partial F_{\nu\lambda}}{\partial x_\mu} + \frac{\partial F_{\lambda\mu}}{\partial x_\nu} = 0$$

$$\epsilon_0 \mu_0 = \frac{1}{c^2}$$

Basic notations and properties

$$x_\mu = (\mathbf{r}, ict), \quad j_\mu = (\mathbf{j}, ic\rho).$$

$$F_{\mu\nu} = \begin{pmatrix} 0 & B_3 & -B_2 & -iE_1/c \\ -B_3 & 0 & -B_1 & -iE_2/c \\ B_2 & -B_1 & 0 & -iE_3/c \\ iE_1/c & iE_2/c & iE_3/c & 0 \end{pmatrix}$$

The antisymmetry of $F_{\mu\nu}$ implies $j_{\mu,\mu} = 0$, i.e.

$$\nabla \mathbf{j} + \frac{\partial \rho}{\partial t} = 0$$

Potentials

$A_\mu = (\mathbf{A}, i\Phi/c)$ – the vector potential.

The homogeneous Maxwell equations become identities if

$$\left. \begin{array}{l} \mathbf{E} = -\nabla\Phi - \frac{\partial \mathbf{A}}{\partial t} \\ \mathbf{B} = \nabla \times \mathbf{A} \end{array} \right\} F_{\mu\nu} = \frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu}$$

The inhomogeneous Maxwell equations:

$$\begin{aligned} \nabla \mathbf{E} = \frac{\rho}{\epsilon_0} &\Rightarrow \Delta \Phi + \frac{\partial}{\partial t} \nabla \mathbf{A} = -\frac{\rho}{\epsilon_0} \\ \nabla \times \mathbf{B} - \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{j} &\Rightarrow \Delta \mathbf{A} - \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla \left(\nabla \mathbf{A} + \frac{1}{c^2} \frac{\partial \Phi}{\partial t} \right) = -\mu_0 \mathbf{j} \end{aligned}$$

Gauge transformation

\mathbf{E} and \mathbf{B} are invariant under the gauge transformation:

$$\left. \begin{array}{l} \mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla\lambda \\ \Phi \rightarrow \Phi' = \Phi - \frac{\partial \lambda}{\partial t} \end{array} \right\} A_\mu \rightarrow A'_\mu = A_\mu + \frac{\partial \lambda}{\partial x_\mu}$$

where $\lambda = \lambda(\mathbf{r}, t)$.

In particular:

$$\frac{\partial A'_\mu}{\partial x_\mu} = \frac{\partial A_\mu}{\partial x_\mu} + \frac{\partial^2 \lambda}{\partial x_\mu^2},$$
$$\nabla \mathbf{A}' = \nabla \mathbf{A} + \Delta \lambda$$

Lorentz gauge

if λ is chosen so that

$$\frac{\partial^2 \lambda}{\partial x_\mu^2} = -\frac{\partial A_\mu}{\partial x_\mu}, \quad \text{i.e.} \quad \square \lambda = -\nabla \mathbf{A} - \frac{1}{c^2} \frac{\partial \Phi}{\partial t}$$

then we get the *Lorentz condition* (manifestly covariant):

$$\frac{\partial A'_\mu}{\partial x_\mu} = 0, \quad \text{i.e.} \quad \nabla \mathbf{A}' + \frac{1}{c^2} \frac{\partial \Phi'}{\partial t} = 0$$

In the Lorentz gauge the Maxwell equations read:

$$\left. \begin{array}{l} \square \Phi' = -\frac{\rho}{\epsilon_0}, \\ \square \mathbf{A}' = -\mu_0 \mathbf{j} \end{array} \right\} \quad \square A'_\mu = -\mu_0 j_\mu$$

Coulomb gauge

if λ is chosen so that $\Delta\lambda = -\nabla\mathbf{A}$

then we get the *Coulomb gauge* (non-covariant) with:

$$\frac{\partial A'_j}{\partial x_j} = 0, \quad \text{i.e.} \quad \nabla\mathbf{A}' = 0 \quad (\text{transversality condition})$$

In the Coulomb gauge the Maxwell equations imply:

$$\begin{aligned} \Delta\Phi &= -\frac{\rho}{\epsilon_0} \Rightarrow \Phi(\mathbf{r}, t) = \frac{1}{4\pi\epsilon_0} \int_V \frac{\rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d^3x' \\ \square\mathbf{A} &= -\mu_0\mathbf{j} + \frac{1}{c^2} \frac{\partial\nabla\Phi}{\partial t} \end{aligned}$$

If $\rho = 0$ then $\Phi = 0$, $\mathbf{B} = \nabla \times \mathbf{A}$, $\mathbf{E} = -\frac{\partial\mathbf{A}}{\partial t}$.

Thus, in the free field ($j_\mu = 0$): $\square\mathbf{A} = 0$.

In the Lorentz gauge, $\rho = 0$ implies $\square\Phi = 0$, then $\Phi \neq 0$.

Therefore, in the following, we shall use the Coulomb gauge.

Lagrangian formulation

$$\frac{\partial \mathcal{L}}{\partial A_\mu} - \frac{\partial}{\partial x_\nu} \left(\frac{\partial \mathcal{L}}{\partial A_{\mu,\nu}} \right) = 0$$

$$\mathcal{L} = -\frac{1}{4\mu_0} F_{\mu\nu} F_{\mu\nu} + j_\mu A_\mu$$

$$F_{\mu\nu} F_{\mu\nu} = 2 (A_{\mu,\nu} A_{\mu,\nu} - A_{\mu,\nu} A_{\nu,\mu})$$

$$\frac{\partial \mathcal{L}}{\partial A_\mu} = \frac{\partial}{\partial A_\mu} j_\sigma A_\sigma = j_\sigma \delta_{\mu\sigma} = j_\mu,$$

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial A_{\mu,\nu}} &= \frac{1}{2\mu_0} \frac{\partial}{\partial A_{\mu,\nu}} (A_{\lambda,\sigma} A_{\sigma,\lambda} - A_{\lambda,\sigma} A_{\lambda,\sigma}) \\ &= \frac{1}{\mu_0} A_{\lambda,\sigma} (\delta_{\lambda\mu} \delta_{\sigma\nu} - \delta_{\lambda\nu} \delta_{\sigma\mu}) = \frac{1}{\mu_0} (A_{\nu,\mu} - A_{\mu,\nu}) = \frac{1}{\mu_0} F_{\mu\nu} \end{aligned}$$

Euler-Lagrange equations: $\boxed{\frac{1}{\mu_0} \frac{\partial F_{\mu\nu}}{\partial x_\nu} = j_\mu}$ – Maxwell equations

Hamiltonian of the electromagnetic field

$$\mathcal{L}_0 = -\frac{1}{4\mu_0} F_{\mu\nu} F_{\mu\nu} = -\frac{1}{2\mu_0} \mathbf{B}^2 + \frac{\epsilon_0}{2} \mathbf{E}^2$$

$$\mathcal{H}_{\text{em}} = \frac{\partial \mathcal{L}_0}{\partial \dot{A}_\mu} \dot{A}_\mu - \mathcal{L}_0 = \frac{\partial \mathcal{L}_0}{\partial A_{\mu,4}} A_{\mu,4} - \mathcal{L}_0$$

$$\frac{\partial \mathcal{L}_0}{\partial A_{\mu,4}} A_{\mu,4} = -\frac{1}{\mu_0} F_{4\mu} A_{\mu,4} = \epsilon_0 \mathbf{E}(\mathbf{E} + \nabla\Phi)$$

$$\mathcal{H}_{\text{em}} = \epsilon_0 \mathbf{E}^2 + \epsilon_0 \mathbf{E}\nabla\Phi + \frac{1}{2\mu_0} \mathbf{B}^2 - \frac{\epsilon_0}{2} \mathbf{E}^2 = \frac{1}{2\mu_0} \mathbf{B}^2 + \frac{\epsilon_0}{2} \mathbf{E}^2 + \epsilon_0 \mathbf{E}\nabla\Phi$$

$$\epsilon_0 \nabla(\mathbf{E}\Phi) = \epsilon_0 \mathbf{E}\nabla\Phi + \rho\Phi.$$

The first term does not contribute to H - it vanishes after the integration.

$$\mathcal{H}_{\text{em}} = \frac{1}{2\mu_0} \mathbf{B}^2 + \frac{\epsilon_0}{2} \mathbf{E}^2 - \rho\Phi$$

Free field: $j_\mu = 0$

$$\mathcal{H}_{\text{em}}^0 = \frac{1}{2\mu_0} \mathbf{B}^2 + \frac{\epsilon_0}{2} \mathbf{E}^2$$

Interaction

$$\mathcal{L}_{\text{int}} = j_\mu A_\mu = \mathbf{j}\mathbf{A} - \rho\Phi$$

$$\mathcal{H}_{\text{int}} = \frac{\partial \mathcal{L}_{\text{int}}}{\partial A_{\mu,4}} A_{\mu,4} - \mathcal{L}_{\text{int}}$$

$$\mathcal{H}_{\text{int}} = -\mathbf{j}\mathbf{A} + \rho\Phi$$

$$\mathcal{H} = \frac{1}{2\mu_0} \mathbf{B}^2 + \frac{\epsilon_0}{2} \mathbf{E}^2 - \mathbf{j}\mathbf{A}$$

For the free field under the Coulomb gauge the only Maxwell equation which is not fulfilled identically is

$$\nabla \times \mathbf{B} - \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} = 0 \Rightarrow \left(\Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \mathbf{A} = 0$$

Let $\mathbf{A}_{\mathbf{k}\alpha}(\mathbf{r}, t) = \boldsymbol{\epsilon}^\alpha e^{i(\mathbf{k}\mathbf{r} - \omega t)}$ then

$$\nabla \mathbf{A}_{\mathbf{k}\alpha} = i(\mathbf{k} \cdot \boldsymbol{\epsilon}^\alpha) \mathbf{A}_{\mathbf{k}\alpha} = 0$$

$$\square \mathbf{A}_{\mathbf{k}\alpha} = \left(-k^2 + \frac{\omega^2}{c^2} \right) \mathbf{A}_{\mathbf{k}\alpha} = 0$$

Thus, the transversality condition implies that the field is transverse, i.e.

$\mathbf{k} \cdot \boldsymbol{\epsilon}^\alpha = 0$. The Maxwell equations are fulfilled if $|k| = \omega/c$

We assume $[\boldsymbol{\epsilon}^{(1)}, \boldsymbol{\epsilon}^{(2)}, \mathbf{k}/|k|]$ form an orthonormal, righthanded system.

The general solution of $\nabla \mathbf{A} = \square \mathbf{A} = 0$: $\mathbf{A} = \sum_{j\alpha} C_j \mathbf{A}_{\mathbf{k}_j\alpha}(\mathbf{r}, t)$.

Plane wave expansion in a cubic box

A complete set of orthogonal periodic functions vanishing at the walls of the box $V = L^3$:

$$\mathbf{u}_{\mathbf{k}\alpha} = \boldsymbol{\epsilon}^{(\alpha)} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad k_1, k_2, k_3 = \frac{2\pi n}{L}, \quad n = \pm 1, \pm 2, \dots$$

$$\begin{aligned} \mathbf{u}_{\mathbf{k}\alpha}^* &= \mathbf{u}_{-\mathbf{k}\alpha}, \\ \frac{1}{V} \int_V \mathbf{u}_{\mathbf{k}\alpha}^* \mathbf{u}_{\mathbf{k}'\alpha'} d^3x &= \delta_{\mathbf{k}\mathbf{k}'} \delta_{\alpha\alpha'}, \\ \frac{1}{V} \int_V \mathbf{u}_{\mathbf{k}\alpha} \mathbf{u}_{\mathbf{k}'\alpha'} d^3x &= \frac{1}{V} \int_V \mathbf{u}_{\mathbf{k}\alpha}^* \mathbf{u}_{\mathbf{k}'\alpha'}^* d^3x = \delta_{\mathbf{k},-\mathbf{k}'} \delta_{\alpha\alpha'} \end{aligned}$$

The vector potential

$$\begin{aligned}\mathbf{A}(\mathbf{r}, t) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \sum_{\alpha} C_{\mathbf{k}\alpha}(t) \boldsymbol{\epsilon}^{(\alpha)} \mathbf{u}_{\mathbf{k}\alpha} \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}}' \sum_{\alpha} \boldsymbol{\epsilon}^{(\alpha)} [C_{\mathbf{k}\alpha}(t) e^{i\mathbf{k}\cdot\mathbf{r}} + C_{\mathbf{k}\alpha}^*(t) e^{-i\mathbf{k}\cdot\mathbf{r}}]\end{aligned}$$

- \mathbf{A} is real,
- \mathbf{A} vanishes at the walls of the box,
- \mathbf{A} fulfils the wave equation $\square\mathbf{A} = 0$ if

$$C_{\mathbf{k}\alpha}(t) = C_{\mathbf{k}\alpha}(0) e^{-i\omega t}, \quad \omega = c|k|.$$

Several identities

$$\Delta \mathbf{A}_{\mathbf{k}\alpha} = -k^2 \mathbf{A}_{\mathbf{k}\alpha}, \quad \frac{\partial}{\partial t} \mathbf{A}_{\mathbf{k}\alpha} = -i\omega \mathbf{A}_{\mathbf{k}\alpha}.$$

$$\int_V (\nabla \times \mathbf{A})^2 d^3\mathbf{r} = - \int_V \mathbf{A} \Delta \mathbf{A} d^3\mathbf{r}$$

Proof:

$$(\nabla \times \mathbf{A}) (\nabla \times \mathbf{A}) = \nabla [\mathbf{A} \times (\nabla \times \mathbf{A})] + \mathbf{A} [\nabla \times (\nabla \times \mathbf{A})],$$

$$\int_V \nabla [\mathbf{A} \times (\nabla \times \mathbf{A})] d^3\mathbf{r} = \int_{S_V} \mathbf{A} (\nabla \times \mathbf{A}) d\boldsymbol{\sigma} = 0,$$

because \mathbf{A} vanishes on S_V ;

$$\mathbf{A} [\nabla \times (\nabla \times \mathbf{A})] = \mathbf{A} [\underbrace{\nabla (\nabla \mathbf{A})}_{=0}] - \mathbf{A} \Delta \mathbf{A}.$$

Hamiltonian of the free field

$$\begin{aligned} H_{\text{em}}^0 &= \int_V \mathcal{H}_{\text{em}}^0 d^3x \\ &= \frac{1}{2} \int_V \left(\frac{1}{\mu_0} \mathbf{B}^2 + \epsilon_0 \mathbf{E}^2 \right) d^3x \\ &= \frac{1}{2} \int_V \left[\frac{1}{\mu_0} (\nabla \times \mathbf{A})^2 + \epsilon_0 \left| \frac{\partial \mathbf{A}}{\partial t} \right|^2 \right] d^3x \\ &= \frac{1}{2} \int_V \left[-\frac{1}{\mu_0} \mathbf{A} \Delta \mathbf{A} + \epsilon_0 \left| \frac{\partial \mathbf{A}}{\partial t} \right|^2 \right] d^3x \end{aligned}$$

Plane wave representation

$$-\frac{1}{\mu_0} \mathbf{A}_{\mathbf{k}'\alpha'} \Delta \mathbf{A}_{\mathbf{k}\alpha} + \epsilon_0 \left| \frac{\partial \mathbf{A}_{\mathbf{k}'\alpha'}}{\partial t} \frac{\partial \mathbf{A}_{\mathbf{k}\alpha}}{\partial t} \right| = \left(\frac{k^2}{\mu_0} + \omega\omega' \right) \mathbf{A}_{\mathbf{k}'\alpha'} \mathbf{A}_{\mathbf{k}\alpha}$$

$$\frac{k^2}{\mu_0} + \omega\omega' = \frac{\omega^2}{c^2 \mu_0} + \omega\omega' \epsilon_0 = \omega(\omega + \omega') \epsilon_0$$

$$H_{\text{em}}^0 = \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'}' \sum_{\alpha\alpha'} \omega(\omega + \omega') \epsilon_0 \mathcal{W}_{\mathbf{k}\mathbf{k}'}^{\alpha\alpha'}$$

$$\begin{aligned} \mathcal{W}_{\mathbf{k}\mathbf{k}'}^{\alpha\alpha'} &= \frac{\delta_{\alpha\alpha'}}{V} \int_V [C_{\mathbf{k}\alpha}(t) e^{i\mathbf{k}\cdot\mathbf{r}} + c.c.] [C_{\mathbf{k}'\alpha'}(t) e^{i\mathbf{k}'\cdot\mathbf{r}} + c.c.] d^3x \\ &= [C_{\mathbf{k}\alpha}^*(t) C_{\mathbf{k}'\alpha'}(t) + C_{\mathbf{k}\alpha}(t) C_{\mathbf{k}'\alpha'}^*(t)] \delta_{\alpha\alpha'} \delta_{\mathbf{k}\mathbf{k}'} \end{aligned}$$

Harmonic mode decomposition

$$H_{\text{em}}^0 = \sum_{\mathbf{k}}' \sum_{\alpha} \omega^2 \epsilon_0 [C_{\mathbf{k}\alpha}^* C_{\mathbf{k}\alpha} + C_{\mathbf{k}\alpha} C_{\mathbf{k}\alpha}^*] = \sum_{\mathbf{k}\alpha} \omega^2 \epsilon_0 C_{\mathbf{k}\alpha}^* C_{\mathbf{k}\alpha}$$

Define:

$$Q_{\mathbf{k}\alpha}(t) = \sqrt{\epsilon_0/2} [C_{\mathbf{k}\alpha}(t) + C_{\mathbf{k}\alpha}^*(t)]$$

$$P_{\mathbf{k}\alpha}(t) = -i\omega\sqrt{\epsilon_0/2} [C_{\mathbf{k}\alpha}(t) - C_{\mathbf{k}\alpha}^*(t)]$$

$$\omega^2 \epsilon_0 C_{\mathbf{k}\alpha}^* C_{\mathbf{k}\alpha} = \frac{1}{2} (P_{\mathbf{k}\alpha}^2 + \omega^2 Q_{\mathbf{k}\alpha}^2)$$

$$H_{\text{em}}^0 = \sum_{\mathbf{k}\alpha} \frac{1}{2} (P_{\mathbf{k}\alpha}^2 + \omega^2 Q_{\mathbf{k}\alpha}^2) \Rightarrow \begin{cases} \frac{\partial H_{\text{em}}^0}{\partial Q_{\mathbf{k}\alpha}} = \omega^2 Q_{\mathbf{k}\alpha} = -\dot{P}_{\mathbf{k}\alpha} \\ \frac{\partial H_{\text{em}}^0}{\partial P_{\mathbf{k}\alpha}} = P_{\mathbf{k}\alpha} = \dot{Q}_{\mathbf{k}\alpha} \end{cases}$$

$$\ddot{Q}_{\mathbf{k}\alpha} + \omega^2 Q_{\mathbf{k}\alpha} = 0$$

QUANTIZATION OF THE ELECTROMAGNETIC FIELD

Field oscillators

Planck \rightarrow Einstein \rightarrow Dirac \rightarrow Feynman

$$P, Q \Rightarrow \hat{P}, \hat{Q}$$

$$\left[\hat{Q}_{\mathbf{k}\alpha}, \hat{P}_{\mathbf{k}'\alpha'} \right] = i\hbar \delta_{\mathbf{k}\mathbf{k}'} \delta_{\alpha\alpha'}, \quad \left[\hat{Q}_{\mathbf{k}\alpha}, \hat{Q}_{\mathbf{k}'\alpha'} \right] = 0, \quad \left[\hat{P}_{\mathbf{k}\alpha}, \hat{P}_{\mathbf{k}'\alpha'} \right] = 0.$$

$$\hat{a}_{\mathbf{k}\alpha} = \frac{1}{\sqrt{2\hbar\omega}} \left(\omega \hat{Q}_{\mathbf{k}\alpha} + i\hat{P}_{\mathbf{k}\alpha} \right)$$

$$\hat{a}_{\mathbf{k}\alpha}^\dagger = \frac{1}{\sqrt{2\hbar\omega}} \left(\omega \hat{Q}_{\mathbf{k}\alpha} - i\hat{P}_{\mathbf{k}\alpha} \right)$$

$$\left[\hat{a}_{\mathbf{k}\alpha}, \hat{a}_{\mathbf{k}'\alpha'}^\dagger \right] = i\hbar \delta_{\mathbf{k}\mathbf{k}'} \delta_{\alpha\alpha'}, \quad \left[\hat{a}_{\mathbf{k}\alpha}, \hat{a}_{\mathbf{k}'\alpha'} \right] = 0, \quad \left[\hat{a}_{\mathbf{k}\alpha}^\dagger, \hat{a}_{\mathbf{k}'\alpha'}^\dagger \right] = 0.$$

The number representation

$$\hat{N} = \sum_{\mathbf{k}\alpha} \hat{N}_{\mathbf{k}\alpha} = \sum_{\mathbf{k}\alpha} \hat{a}_{\mathbf{k}\alpha}^\dagger \hat{a}_{\mathbf{k}\alpha}$$

$$\hat{H}_{\text{em}}^0 = \sum_{\mathbf{k}\alpha} \frac{1}{2} \left(\hat{P}_{\mathbf{k}\alpha}^2 + \omega^2 \hat{Q}_{\mathbf{k}\alpha}^2 \right) = \frac{1}{2} \sum_{\mathbf{k}\alpha} \hbar\omega \left(\hat{a}_{\mathbf{k}\alpha}^\dagger \hat{a}_{\mathbf{k}\alpha} + \hat{a}_{\mathbf{k}\alpha} \hat{a}_{\mathbf{k}\alpha}^\dagger \right)$$

$$\hat{H}_{\text{em}}^0 = \sum_{\mathbf{k}\alpha} \hbar\omega \left(\hat{N}_{\mathbf{k}\alpha} + \frac{1}{2} \right)$$

$$\hat{H}_{\text{em}}^0 |n_{\mathbf{k}_1\alpha_1} n_{\mathbf{k}_2\alpha_2} \cdots n_{\mathbf{k}_j\alpha_j} \cdots\rangle = E_{12\dots j\dots} |n_{\mathbf{k}_1\alpha_1} n_{\mathbf{k}_2\alpha_2} \cdots n_{\mathbf{k}_j\alpha_j} \cdots\rangle$$

$$E_{12\dots j\dots} = \sum_j \hbar\omega_j \left(n_{\mathbf{k}_j\alpha_j} + \frac{1}{2} \right)$$

The energy of the vacuum

$$\hat{N}|n_{\mathbf{k}_1\alpha_1}n_{\mathbf{k}_2\alpha_2}\cdots\rangle = N|n_{\mathbf{k}_1\alpha_1}n_{\mathbf{k}_2\alpha_2}\cdots\rangle, \quad N = \sum_j n_{\mathbf{k}_j\alpha_j}$$

$$\hat{N}|0\rangle = 0$$

$$\hat{H}_{\text{em}}^0|0\rangle = E_0|0\rangle, \quad E_0 = \frac{1}{2} \sum_j \hbar\omega_j$$

One can shift the energy scale so that the energy of the vacuum is equal to 0:

$$\hat{H}^{\text{EM}} = \hat{H}_{\text{em}}^0 - E_0 = \sum_j \hbar\omega_j \hat{N}_{\mathbf{k}_j\alpha_j}$$

$$E_{12\dots j\dots}^{\text{EM}} = \sum_j \hbar\omega_j n_{\mathbf{k}_j\alpha_j}$$

$$\hat{H}^{\text{EM}}|0\rangle = 0$$

TIME EVOLUTION OF THE CREATION OPERATORS

$$\dot{\hat{a}}_{\mathbf{k}\alpha} = \frac{1}{i\hbar} [\hat{a}_{\mathbf{k}\alpha}, \hat{H}] = -i\omega \hat{a}_{\mathbf{k}\alpha}$$

$$\hat{a}_{\mathbf{k}\alpha}(t) = \hat{a}_{\mathbf{k}\alpha}(0)e^{-i\omega t}$$

The annihilation operators: Hermitian conjugate, i.e.

$$\hat{a}_{\mathbf{k}\alpha}(t)^\dagger = \hat{a}_{\mathbf{k}\alpha}(0)^\dagger e^{i\omega t}$$

MOMENTUM OF THE FIELD – THE POYNTING VECTOR

$$\hat{\mathbf{P}} = \int_V \hat{\mathbf{E}} \times \hat{\mathbf{B}} d^3x = \sum_{\mathbf{k}\alpha} \hbar \mathbf{k} \left(N_{\mathbf{k}\alpha} + \frac{1}{2} \right) = \sum_{\mathbf{k}\alpha} \hbar \mathbf{k} N_{\mathbf{k}\alpha}$$

because $\sum_{\mathbf{k}} \mathbf{k} = 0$ – the terms \mathbf{k} and $-\mathbf{k}$ cancel each other.

THE MASS OF A PHOTON

$$\hat{H}|1\rangle = \hbar\omega \left(1 + \frac{1}{2}\right) |1\rangle = E|1\rangle \Rightarrow E = \frac{3}{2}\hbar\omega$$

$$\hat{\mathbf{P}}|1\rangle = \hbar\mathbf{k} \left(1 + \frac{1}{2}\right) |1\rangle = \mathbf{p}|1\rangle \Rightarrow \mathbf{p} = \frac{3}{2}\hbar\mathbf{k}$$

$$m^2c^4 = E^2 - p^2c^2 = \frac{9}{4}\hbar^2 (\omega^2 - k^2c^2) = 0$$

because $\omega = kc$

Conclusion: $m = 0$ (the mass of a photon is equal to 0)

SPIN OF A PHOTON

The radiation field is transverse: $\nabla \mathbf{A} = 0$.

The transversality condition implies that $\mathbf{k}\epsilon^\alpha = 0$ – the polarization vectors ϵ^α are perpendicular to the direction \mathbf{k} of the propagation.

Spin emerges as the generator of the infinitesimal rotation around the direction of the propagation:

$$\begin{pmatrix} \epsilon^{(1)'} \\ \epsilon^{(2)'} \end{pmatrix} = \begin{pmatrix} 1 & -\delta\varphi \\ \delta\varphi & 1 \end{pmatrix} \begin{pmatrix} \epsilon^{(1)} \\ \epsilon^{(2)} \end{pmatrix} = \begin{pmatrix} \epsilon^{(1)} - \epsilon^{(2)}\delta\varphi \\ \epsilon^{(2)} - \epsilon^{(1)}\delta\varphi \end{pmatrix}$$

Let $\epsilon^\pm = \frac{1}{\sqrt{2}} (\epsilon^{(1)} \pm i\epsilon^{(2)})$ – the circular (helicity) basis

Then

$$\epsilon^{\pm'} = \epsilon^\pm \pm i\epsilon^\pm\delta\varphi = \left(1 + \frac{i}{\hbar} S_z \delta\varphi\right) \epsilon^\pm,$$

Conclusion: $S_z = m\hbar$, $m = \pm 1$
 $m = 0$ is absent!

Spin of the photon may be either parallel or antiparallel to the direction of the propagation (positive or negative helicity). The absence of helicity zero is a consequence of the zero mass. The restriction of the helicity to its maximum and minimum possible values is a general property of all massless particles (e.g. the massless neutrino).

The orthogonality conditions:

$$\boldsymbol{\epsilon}^{\pm} \cdot \boldsymbol{\epsilon}^{\pm*} = 1, \quad \boldsymbol{\epsilon}^{\pm} \cdot \boldsymbol{\epsilon}^{\mp*} = 0, \quad \mathbf{k} \cdot \boldsymbol{\epsilon}^{\pm} = 0$$

Creation and annihilation operators of the circularly polarized (i.e. of defined helicity) states:

$$\hat{a}_{\mathbf{k},\pm}^\dagger = \frac{1}{\sqrt{2}} \left(\hat{a}_{\mathbf{k},1}^\dagger \mp i\hat{a}_{\mathbf{k},2}^\dagger \right)$$

Spin operator:

$$\hat{\mathbf{M}}_{\text{spin}} = \sum_{\mathbf{k}} \mathbf{k} \left(\hat{a}_{\mathbf{k},+}^\dagger \hat{a}_{\mathbf{k},+} - \hat{a}_{\mathbf{k},-}^\dagger \hat{a}_{\mathbf{k},-} \right) = \sum_{\mathbf{k}} \mathbf{k} \left(\hat{N}_{\mathbf{k},+} - \hat{N}_{\mathbf{k},-} \right)$$

$$\hat{a}_1 = \frac{1}{\sqrt{2}} (\hat{a}_+ - \hat{a}_-), \quad \hat{a}_2 = \frac{i}{\sqrt{2}} (\hat{a}_+ + \hat{a}_-)$$

Massive particles: $m_s = -s, -s + 1, \dots, +s$

Massless particles: $m_s = -s, +s$

INTERACTIONS

Transverse and longitudinal components of the e-m field

$$\mathbf{E} = \mathbf{E}_{\perp} + \mathbf{E}_{\parallel} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\Phi$$

Transverse component: $\nabla\mathbf{E}_{\perp} = 0, \quad \mathbf{E}_{\perp} = -\frac{\partial \mathbf{A}}{\partial t}$

Longitudinal component: $\nabla \times \mathbf{E}_{\parallel} = 0, \quad \mathbf{E}_{\parallel} = -\nabla\Phi$

$$\int_V \mathbf{E}^2 d^3x = \int_V \left(\mathbf{E}_{\perp}^2 + \mathbf{E}_{\parallel}^2 \right) d^3x + 2 \underbrace{\int_V \mathbf{E}_{\perp} \mathbf{E}_{\parallel} d^3x}_{=0}$$

$$\int_V \mathbf{E}_{\perp} \mathbf{E}_{\parallel} d^3x = - \int_V \mathbf{E}_{\perp} \nabla\Phi d^3x = \int_V \Phi \nabla\mathbf{E}_{\perp} d^3x = 0$$

$$\int_V \mathbf{E}_{\parallel}^2 d^3x = - \int_V \mathbf{E}_{\parallel} \nabla\Phi d^3x = \int_V \Phi \nabla\mathbf{E}_{\parallel}^2 d^3x = \frac{1}{\epsilon_0} \int_V \Phi \rho d^3x$$

Hamiltonian

$$\begin{aligned} H &= \int_V \mathcal{H} d^3x = \int_V (\mathcal{H}_{\text{em}}^0 + \mathcal{H}_{\text{int}}) d^3x \\ &= \int_V \left(\frac{1}{2\mu_0} \mathbf{B}^2 + \frac{\epsilon_0}{2} \mathbf{E}_{\perp}^2 \right) d^3x + \int_V \left(\frac{1}{2} \Phi \rho - \mathbf{j} \mathbf{A} \right) d^3x \\ &= H_{\text{em}}^0 + \frac{1}{2} \int_V \frac{\rho(\mathbf{r}, t) \rho(\mathbf{r}', t)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3x d^3x' - \int_V \mathbf{j} \mathbf{A} d^3x \end{aligned}$$

Point charges: $\rho(\mathbf{r}) = \sum_i e_i \delta(\mathbf{r} - \mathbf{r}_i)$

$$\begin{aligned} \frac{1}{2} \int_V \frac{\rho(\mathbf{r}, t) \rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d^3x d^3x' &= \frac{1}{2} \sum_{i,j} \frac{e_i e_j}{|\mathbf{r}_i - \mathbf{r}_j|} \\ &= \sum_{j < i} \frac{e_i e_j}{r_{ij}} + \underbrace{\frac{1}{2} \sum_i \frac{e_i^2}{|\mathbf{r}_i - \mathbf{r}_i|}}_{\text{self-interaction}} \end{aligned}$$

Schrödinger field + Maxwell field:

$$H = H_{\text{particles}} + H_{\text{em}} + H_{\text{int}}$$

$$i\hbar \frac{\partial \psi}{\partial t} \Rightarrow i\hbar \frac{\partial \psi}{\partial t} - e\Phi\psi$$

$$i\hbar \nabla \Rightarrow i\hbar \nabla + e\mathbf{A}\psi$$

From here

$$\rho = e\psi^*\psi$$

$$\mathbf{j} = \frac{e\hbar}{2im} (\psi^* \nabla \psi - \nabla \psi^* \psi) - \frac{e^2}{m} \mathbf{A} \psi^* \psi$$

These substitutions generate $-\int_V \mathbf{j} \cdot \mathbf{A} d^3x$

The Hamiltonian density:

$$\begin{aligned}\mathcal{H}_{\text{particles}} &= \\ [A_\mu = 0] &= \frac{\hbar^2}{2m} \nabla\psi^* \nabla\psi + V(\mathbf{r}) \psi^* \psi \\ &= \frac{1}{2m} (i\hbar\nabla\psi^*) (-i\hbar\nabla\psi) + V(\mathbf{r}) \psi^* \psi \\ [A_\mu \neq 0] &\Rightarrow \frac{1}{2m} (i\hbar\nabla\psi^* - e\mathbf{A}\psi^*) (-i\hbar\nabla\psi - e\mathbf{A}\psi) + V(\mathbf{r}) \psi^* \psi \\ \\ \mathcal{H}_{\text{em}}^0 &= \frac{1}{2\mu_0} \mathbf{B}^2 + \frac{\epsilon_0}{2} \mathbf{E}_\perp^2 \\ &= \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 + \frac{\epsilon_0}{2} \left| \frac{\partial \mathbf{A}}{\partial t} \right|^2\end{aligned}$$

The Hamiltonian:

$$\begin{aligned} H &= \int_V \left[\frac{1}{2m} (i\hbar\nabla\psi^* - e\mathbf{A}\psi^*) (-i\hbar\nabla\psi - e\mathbf{A}\psi) + V(\mathbf{r}) \psi^*\psi \right] d^3x \\ &+ \frac{1}{2} \int_V \left[\frac{1}{\mu_0} (\nabla \times \mathbf{A})^2 + \epsilon_0 \left| \frac{\partial \mathbf{A}}{\partial t} \right|^2 \right] d^3x \\ &+ \frac{1}{2} \int_V \int_{V'} \frac{\rho(\mathbf{r}', t)\rho(\mathbf{r}, t)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3x d^3x' \end{aligned}$$

QUANTIZATION

$$\text{bozons:} \quad [\hat{a}_q, \hat{a}_{q'}] = [\hat{a}_q^\dagger, \hat{a}_{q'}^\dagger] = 0, \quad [\hat{a}_q, \hat{a}_{q'}^\dagger] = \delta_{qq'}$$

$$\text{fermions:} \quad \{\hat{a}_q, \hat{a}_{q'}\} = \{\hat{a}_q^\dagger, \hat{a}_{q'}^\dagger\} = 0, \quad \{\hat{a}_q, \hat{a}_{q'}^\dagger\} = \delta_{qq'}$$

$$\hat{\rho} \hat{\rho}' = e^2 \hat{\psi}^\dagger \hat{\psi} \hat{\psi}'^\dagger \hat{\psi}' = e^2 \hat{\psi}^\dagger \hat{\psi}'^\dagger \hat{\psi}' \hat{\psi} + \underbrace{e^2 \hat{\psi}^\dagger \hat{\psi}' \delta(\mathbf{r} - \mathbf{r}')}_{\text{self-interaction}}$$

$$\hat{H} = \hat{H}_0 + \hat{H}'$$

\hat{H}_0 – free fields

\hat{H}' – interactions

THE HAMILTONIAN

$$\begin{aligned}
 \hat{H}_0 &= \int_V \left[\frac{\hbar^2}{2m} \nabla \hat{\psi}^\dagger \nabla \hat{\psi} + V(\mathbf{r}) \hat{\psi}^\dagger \hat{\psi} + \frac{1}{2\mu_0} (\nabla \times \mathbf{A})^2 + \frac{\epsilon_0}{2} \left| \frac{\partial \mathbf{A}}{\partial t} \right|^2 \right] d^3x \\
 &= \sum_j \hat{N}_j \mathcal{E}_j + \sum_{\mathbf{k}\alpha} \left(\hat{N}_{\mathbf{k}\alpha} + \frac{1}{2} \right)
 \end{aligned}$$

$$\begin{aligned}
 \hat{H}' &= \int_V \left[\frac{ie\hbar}{2m} \left(\hat{\mathbf{A}} \hat{\psi}^\dagger \nabla \hat{\psi} - (\nabla \hat{\psi}^\dagger) \hat{\mathbf{A}} \hat{\psi} \right) + \frac{e^2}{2m} \hat{\mathbf{A}} \hat{\psi}^\dagger \hat{\mathbf{A}} \hat{\psi} \right] d^3x \\
 &+ \frac{e^2}{2} \int_V \int_{V'} \frac{\hat{\psi}^\dagger \hat{\psi}'^\dagger \hat{\psi}' \hat{\psi}}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3x d^3x'
 \end{aligned}$$

THE COULOMB INTERACTION

The radiation field is neglected ($\mathbf{A} = 0$).

The unperturbed problem corresponds to a system of non-interacting particles

$$\hat{\psi}(\mathbf{r}, t) = \sum_k \hat{a}_k(t) u_k(\mathbf{r}), \quad \hat{\psi}(\mathbf{r}, t)^\dagger = \sum_k \hat{a}_k^\dagger(t) u_k^*(\mathbf{r})$$

$$\left(-\frac{\hbar^2}{2m} \Delta + V \right) u_k = \mathcal{E}_k u_k$$

$$\hat{H}_0 = \sum_k \mathcal{E}_k \hat{a}_k^\dagger \hat{a}_k = \sum_k \mathcal{E}_k \hat{N}_k$$

$$\hat{H}_0 |n_1, n_2, \dots, n_k, \dots\rangle = E_{n_1, n_2, \dots, n_k, \dots}^0 |n_1, n_2, \dots, n_k, \dots\rangle$$

$$E_{n_1, n_2, \dots, n_k, \dots}^0 = \sum_k n_k \mathcal{E}_k$$

The basis:

$$\hat{N}_k |n_1, n_2, \dots, n_k, \dots\rangle = n_k |n_1, n_2, \dots, n_k, \dots\rangle$$

bosons:

$$\hat{a}_k |n_1, n_2, \dots, n_k, \dots\rangle = \sqrt{n_k} |n_1, n_2, \dots, n_k - 1, \dots\rangle$$

$$\hat{a}_k^\dagger |n_1, n_2, \dots, n_k, \dots\rangle = \sqrt{n_k + 1} |n_1, n_2, \dots, n_k + 1, \dots\rangle$$

fermions:

$$\hat{a}_k |n_1, n_2, \dots, n_k, \dots\rangle = \Theta_k n_k |n_1, n_2, \dots, 1 - n_k, \dots\rangle$$

$$\hat{a}_k^\dagger |n_1, n_2, \dots, n_k, \dots\rangle = \Theta_k (1 - n_k) |n_1, n_2, \dots, 1 - n_k, \dots\rangle$$

$$\Theta_k = \pm 1$$

The perturbation

$$\hat{H}' = \frac{e^2}{2} \int_V \int_{V'} \frac{\hat{\psi}^\dagger \hat{\psi}'^\dagger \hat{\psi}' \hat{\psi}}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3x d^3x' = \frac{1}{2} \sum_{jklm} \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_m \langle jk|lm \rangle$$

$$\underbrace{\langle jk|lm \rangle}_{\text{'physical'}} = \frac{e^2}{4\pi\epsilon_0} \int_V \int_{V'} \frac{u_j^* u_k'^* u_l' u_m}{|\mathbf{r} - \mathbf{r}'|} d^3x d^3x' \equiv \underbrace{(jm|kl)}_{\text{notation}}$$

'physical' \Leftarrow notation \Rightarrow 'chemical' (Mulliken)

$$\left. \begin{aligned} \langle kk|kk \rangle &= \frac{e^2}{4\pi\epsilon_0} \int_V \int_{V'} \frac{|u_k|^2 |u_k'|^2}{|\mathbf{r} - \mathbf{r}'|} d^3x d^3x' \\ \langle kl|lk \rangle &= \frac{e^2}{4\pi\epsilon_0} \int_V \int_{V'} \frac{|u_k|^2 |u_l'|^2}{|\mathbf{r} - \mathbf{r}'|} d^3x d^3x' \\ \langle kl|kl \rangle &= \frac{e^2}{4\pi\epsilon_0} \int_V \int_{V'} \frac{u_k^* u_l'^* u_k' u_l}{|\mathbf{r} - \mathbf{r}'|} d^3x d^3x' \end{aligned} \right\} \begin{array}{l} \text{Coulomb integrals} \\ \text{Exchange integrals} \end{array}$$

The Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{H}' = \sum_k \hat{a}_k^\dagger \hat{a}_k \mathcal{E}_k + \frac{1}{2} \sum_{jklm} \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_m \langle jk|lm \rangle$$

Bozons

- One occupied state ($n_j = 0$ if $j \neq k$)

$$\hat{a}_k^\dagger \hat{a}_k^\dagger \hat{a}_k \hat{a}_k = \hat{a}_k^\dagger (\hat{a}_k \hat{a}_k \hat{a}_k^\dagger - 1) \hat{a}_k = \hat{N}_k^2 - \hat{N}_k$$

$$\begin{aligned} E_k &= E_k^0 + \langle n_k | \hat{H}' | n_k \rangle \\ &= n_k \mathcal{E}_k + \frac{1}{2} n_k (n_k - 1) \langle kk | kk \rangle \end{aligned}$$

- Two occupied states ($n_j = 0$ if $j \neq k, l$)

$$\hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_k \hat{a}_l = \hat{a}_l^\dagger \hat{a}_k^\dagger \hat{a}_k \hat{a}_l = \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_l \hat{a}_k = \hat{a}_l^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_k = \hat{N}_k \hat{N}_l$$

$$\begin{aligned} E_{kl} &= E_{kl}^0 + \langle n_k n_l | \hat{H}' | n_k n_l \rangle \\ &= n_k \mathcal{E}_k + n_l \mathcal{E}_l + n_k n_l [\langle kl | lk \rangle + \langle kl | kl \rangle] \end{aligned}$$

Fermions

Two occupied states: $n_k = n_l = 1$, $n_j = 0$ if $j \neq k, l$)

$$\hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_k \hat{a}_l = \hat{a}_l^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_k = -\hat{N}_k \hat{N}_l$$

$$\hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_l \hat{a}_k = \hat{a}_l^\dagger \hat{a}_k^\dagger \hat{a}_k \hat{a}_l = \hat{N}_k \hat{N}_l$$

$$\begin{aligned} E_{kl} &= E_{kl}^0 + \langle n_k n_l | \hat{H}' | n_k n_l \rangle \\ &= \mathcal{E}_k + \mathcal{E}_l + \langle kl | lk \rangle - \langle kl | kl \rangle \end{aligned}$$

In the case of bosons the exchange energy is positive;
in the case of fermions it is negative.

THE THEORY OF RADIATION

The Coulomb interaction is neglected ($\Phi = 0$).

$$\hat{H}_0 = \hat{H}_{01} + \hat{H}_{02} = \sum_j \hat{N}_j \mathcal{E}_j + \sum_{\mathbf{k}\alpha} \left(\hat{N}_{\mathbf{k}\alpha} + \frac{1}{2} \right)$$

$$\hat{H}' = \int_V \left[\frac{ie\hbar}{2m} \left(\hat{\mathbf{A}}\hat{\psi}^\dagger \nabla \hat{\psi} - (\nabla \hat{\psi}^\dagger) \hat{\mathbf{A}}\hat{\psi} \right) + \frac{e^2}{2m} \hat{\mathbf{A}}\hat{\psi}^\dagger \hat{\mathbf{A}}\hat{\psi} \right] d^3x$$

$$\begin{aligned} - \int_V (\nabla \hat{\psi}^\dagger) \hat{\mathbf{A}}\hat{\psi} d^3x &= \underbrace{- \int_{S_V} \nabla(\hat{\psi}^\dagger \hat{\mathbf{A}}\hat{\psi}) d\boldsymbol{\sigma}}_{=0} + \int_V \hat{\psi}^\dagger \nabla(\hat{\mathbf{A}}\hat{\psi}) d^3x \\ &= \int_V \hat{\psi}^\dagger \underbrace{(\nabla \hat{\mathbf{A}})}_{=0} \hat{\psi} d^3x + \int_V \hat{\psi}^\dagger \hat{\mathbf{A}} \nabla \hat{\psi} d^3x \end{aligned}$$

$$\hat{H}' = \frac{ie\hbar}{m} \int_V \hat{\mathbf{A}} \hat{\psi}^\dagger \nabla \hat{\psi} d^3x + \frac{e^2}{2m} \int_V \hat{\psi}^\dagger |\hat{\mathbf{A}}|^2 \hat{\psi} d^3x$$

We are interested in the single-photon radiative processes only. Therefore the second term does not contribute and

$$\hat{H}' = \frac{ie\hbar}{m} \int_V \hat{\mathbf{A}} \hat{\psi}^\dagger \nabla \hat{\psi} d^3x$$

$$\hat{a}_m(t) = \frac{1}{i\hbar} [\hat{a}_m, \hat{H}_{01}] = \frac{1}{i\hbar} \sum_j \underbrace{[\hat{a}_m, \hat{a}_j^\dagger]}_{=\delta_{mj}} \hat{a}_j \mathcal{E}_j = -\frac{i}{\hbar} \mathcal{E}_m \hat{a}_m(t)$$

$$\hat{a}_m(t) = e^{-\frac{i}{\hbar} \mathcal{E}_m t} \hat{a}_m(0)$$

We denote hereafter $\hat{a}(0) \equiv \hat{a}$.

Several formulas:

$$\hat{\psi}(\mathbf{r}, t) = \sum_j \hat{a}_j(t) u_j(\mathbf{r}) = \sum_j \hat{a}_j u_j(\mathbf{r}) e^{-\frac{i}{\hbar} \mathcal{E}_j t}$$

$$\hat{\psi}^\dagger \nabla \hat{\psi} = \sum_{jl} \hat{a}_j^\dagger \hat{a}_l e^{\frac{i}{\hbar} (\mathcal{E}_j - \mathcal{E}_l) t} u_j^*(\mathbf{r}) \nabla u_l(\mathbf{r})$$

$$\begin{aligned} \mathbf{A}(\mathbf{r}, t) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}}' \sum_{\alpha} \boldsymbol{\epsilon}^{(\alpha)} \left[\hat{C}_{\mathbf{k}\alpha} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} + \hat{C}_{\mathbf{k}\alpha}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega t)} \right] \\ &= \sqrt{\frac{\hbar}{2\epsilon_0 V}} \sum_{\mathbf{k}}' \sum_{\alpha} \frac{\boldsymbol{\epsilon}^{(\alpha)}}{\sqrt{\omega}} \left[\hat{a}_{\mathbf{k}\alpha} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} + \hat{a}_{\mathbf{k}\alpha}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega t)} \right] \end{aligned}$$

$$\begin{aligned}
& \int_V \hat{\mathbf{A}} \hat{\psi}^\dagger \nabla \hat{\psi} d^3x \\
= & \sqrt{\frac{\hbar}{2\epsilon_0 V}} \sum'_{\mathbf{k}\alpha} \sum_{jl} \frac{1}{\sqrt{\omega}} \left[\hat{a}_{\mathbf{k}\alpha} \hat{a}_j^\dagger \hat{a}_l e^{i\omega_- t} M_{jl}^{\mathbf{k}\alpha} + \hat{a}_{\mathbf{k}\alpha}^\dagger \hat{a}_j^\dagger \hat{a}_l e^{i\omega_+ t} M_{jl}^{-\mathbf{k}\alpha} \right]
\end{aligned}$$

$$\omega_{\pm} \equiv \frac{\mathcal{E}_j - \mathcal{E}_l}{\hbar} \pm \omega, \quad \omega = kc$$

$$M_{jl}^{\mathbf{k}\alpha} = \int_V u_j^* \boldsymbol{\epsilon}^{(\alpha)} e^{i\mathbf{k}\mathbf{r}} \nabla u_l d^3x$$

$$\langle B | \hat{H}' | A \rangle = \frac{ie\hbar}{m} \langle B | \int_V \hat{\mathbf{A}} \hat{\psi}^\dagger \nabla \hat{\psi} d^3x | A \rangle = \frac{ie\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V}} \sum'_{\mathbf{k}\alpha} \sum_{jl} \frac{1}{\sqrt{\omega}}$$

$$\left[\langle B | \hat{a}_{\mathbf{k}\alpha} \hat{a}_j^\dagger \hat{a}_l | A \rangle e^{i\omega_- t} M_{jl}^{\mathbf{k}\alpha} + \langle B | \hat{a}_{\mathbf{k}\alpha}^\dagger \hat{a}_j^\dagger \hat{a}_l | A \rangle e^{i\omega_+ t} M_{jl}^{-\mathbf{k}\alpha} \right]$$

One-electron system + radiation field

Transition from: $|A\rangle = |E_a; n_{\mathbf{k}_1\alpha_1} n_{\mathbf{k}_2\alpha_2} \cdots n_{\mathbf{k}_p\alpha_p} \cdots\rangle,$

to: $|K\rangle = \sum_B C_B |B\rangle$

$$|B\rangle = |E_b; n_{\mathbf{k}_1\alpha_1} n_{\mathbf{k}_2\alpha_2} \cdots n'_{\mathbf{k}_p\alpha_p} \cdots\rangle.$$

Short-hand notation (only one photonic occupation number is changed):

$$|A\rangle = |E_a; n_{\mathbf{k}\alpha}\rangle,$$

$$|B\rangle = |E_b; n'_{\mathbf{k}\alpha}\rangle$$

where $n_{\mathbf{k}\alpha} \equiv n_{\mathbf{k}_p\alpha_p}$

Transition probability is given as the first-order perturbation:

$$W_{A \rightarrow B} \sim |C_B|^2 \sim |\langle B | \hat{H}' | A \rangle|^2$$

Absorption

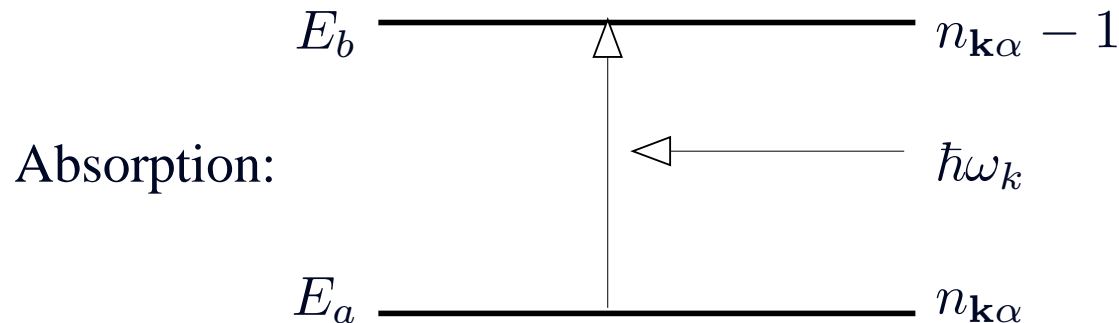
$$\hat{a}_{\mathbf{k}\alpha} \hat{a}_j^\dagger \hat{a}_l |A\rangle = \hat{a}_{\mathbf{k}\alpha} \hat{a}_j^\dagger \hat{a}_l |E_a; n_{\mathbf{k}\alpha}\rangle = \delta_{al} \sqrt{n_{\mathbf{k}\alpha}} |E_j; n_{\mathbf{k}\alpha} - 1\rangle$$

$$\langle B | \hat{a}_{\mathbf{k}\alpha} \hat{a}_j^\dagger \hat{a}_l |A\rangle = \delta_{al} \sqrt{n_{\mathbf{k}\alpha}} \langle E_b; n'_{\mathbf{k}\alpha} | E_j; n_{\mathbf{k}\alpha} - 1\rangle = \delta_{al} \delta_{bj} \delta(n'_{\mathbf{k}\alpha}, n_{\mathbf{k}\alpha} - 1) \sqrt{n_{\mathbf{k}\alpha}}$$

Thus, the matrix element vanishes unless

$$|A\rangle = |E_a; n_{\mathbf{k}\alpha}\rangle, \quad \text{and} \quad |B\rangle = |E_b; n_{\mathbf{k}\alpha} - 1\rangle,$$

i.e. in the final state there is one photon less than in the initial one:



Emission

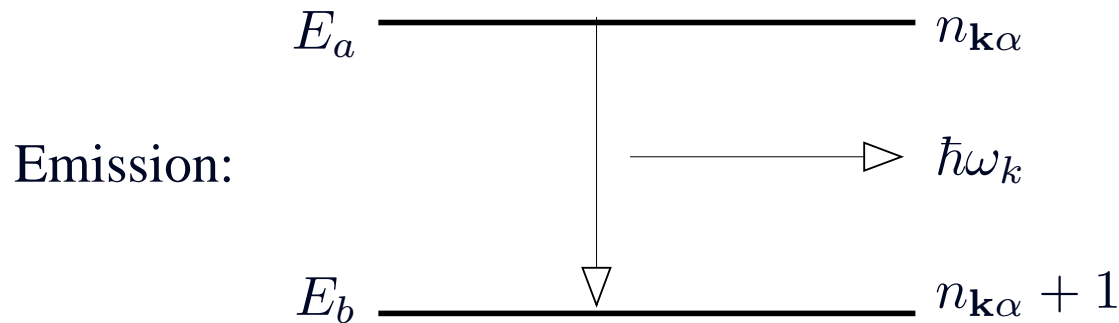
$$\hat{a}_{\mathbf{k}\alpha}^\dagger \hat{a}_j^\dagger \hat{a}_l |A\rangle = \hat{a}_{\mathbf{k}\alpha}^\dagger \hat{a}_j^\dagger \hat{a}_l |E_a; n_{\mathbf{k}\alpha}\rangle = \delta_{al} \sqrt{n_{\mathbf{k}\alpha} + 1} |E_j; n_{\mathbf{k}\alpha} + 1\rangle$$

$$\langle B | \hat{a}_{\mathbf{k}\alpha}^\dagger \hat{a}_j^\dagger \hat{a}_l |A\rangle = \delta_{al} \sqrt{n_{\mathbf{k}\alpha} + 1} \langle E_b; n'_{\mathbf{k}\alpha} | E_j; n_{\mathbf{k}\alpha} + 1\rangle = \delta_{al} \delta_{bj} \delta(n'_{\mathbf{k}\alpha}, n_{\mathbf{k}\alpha} + 1) \sqrt{n_{\mathbf{k}\alpha} + 1}$$

Thus, the matrix element vanishes unless

$$|A\rangle = |E_a; n_{\mathbf{k}\alpha}\rangle, \quad \text{and} \quad |B\rangle = |E_b; n_{\mathbf{k}\alpha} + 1\rangle,$$

i.e. in the final state there is one photon more than in the initial one:



Transition probability

$$\langle B|\hat{H}'|A\rangle = \frac{ie\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V}} \begin{cases} \sqrt{\frac{n_{\mathbf{k}\alpha}}{\omega}} M_{ba}^{\mathbf{k}\alpha} e^{i\omega-t}, & \text{if } n'_{\mathbf{k}\alpha} = n_{\mathbf{k}\alpha} - 1 \\ \sqrt{\frac{n_{\mathbf{k}\alpha} + 1}{\omega}} M_{ba}^{-\mathbf{k}\alpha} e^{i\omega+t}, & \text{if } n'_{\mathbf{k}\alpha} = n_{\mathbf{k}\alpha} + 1 \end{cases}$$

$$W_{A \rightarrow B} = \frac{1}{\hbar^2} \sum_{\mathbf{k}\alpha} \frac{1}{t} \left| \int_0^t \langle B|\hat{H}'|A\rangle dt \right|^2$$

$$\frac{1}{t} \left| \int_0^t e^{i\omega t} dt \right|^2 = \frac{|e^{i\omega t} - 1|^2}{t\omega^2} = \frac{\sin^2 t\omega/2}{t(\omega/2)^2} \xrightarrow{t \rightarrow \infty} \pi\delta(\omega/2) = 2\pi\delta(\omega)$$

Transition probability

$$W_{A \rightarrow B} = \frac{e^2 \hbar}{2m^2 \epsilon_0 V} \sum_{\mathbf{k}\alpha} \begin{cases} \frac{n_{\mathbf{k}\alpha}}{\omega} |M_{ba}^{\mathbf{k}\alpha}|^2 \delta(\omega_-) \\ \frac{n_{\mathbf{k}\alpha} + 1}{\omega} |M_{ba}^{-\mathbf{k}\alpha}|^2 \delta(\omega_+) \end{cases}$$

$$\omega_- = \frac{E_b - E_a}{\hbar} - \omega, \Rightarrow \delta(\omega_-) \Rightarrow \omega = \frac{E_b - E_a}{\hbar} = kc - \text{absorption}$$

$$\omega_+ = \frac{E_b - E_a}{\hbar} + \omega, \Rightarrow \delta(\omega_+) \Rightarrow \omega = \frac{E_a - E_b}{\hbar} = kc - \text{emission}$$

$$E_b = E_a \pm \hbar\omega - \text{energy conservation}$$

Absorption and induced (stimulated) emission

Radiative processes in the presence of the radiation field, i.e. when $n_{\mathbf{k}\alpha} > 0$. Let us assume that $n_{\mathbf{k}\alpha} \gg 1$. Then $n_{\mathbf{k}\alpha} \rightarrow n(\omega)$.

$n(\omega)d\omega$ — the number of photons in $\langle \omega, \omega + d\omega \rangle$

$\frac{\hbar\omega}{V}$ — the contribution of one photon to the density of energy

$c \frac{\hbar\omega}{V}$ — the contribution of one photon to the intensity $I(\omega)$ of radiation

Then, for a fixed polarization,

$$\sum_{\mathbf{k}} (\dots) n_{\mathbf{k}\alpha} \Rightarrow \int (\dots) n(\omega) d\omega = \int (\dots) \frac{I(\omega)}{c(\hbar\omega/V)} d\omega$$

because
$$n(\omega)d\omega = \frac{I(\omega)}{c(\hbar\omega/V)} d\omega$$

Absorption and induced (stimulated) emission

$$W_{A \rightarrow B}^{\text{ind}} = \frac{2\pi h \alpha_o}{m^2} \int_{-\infty}^{\infty} \frac{I(\omega)}{\omega^2} |M_{ba}^{\pm \mathbf{k} \alpha}|^2 \delta(\omega_{\mp}) d\omega$$

$$= \frac{2\pi h \alpha_o}{m^2} \frac{I(\omega_{ba})}{\omega_{ba}^2} |M_{ba}^{\pm \mathbf{k}_{ba} \alpha}|^2$$

$$\omega_{ba} = \pm \frac{E_b - E_a}{\hbar} = c k_{ba}$$

$$M_{ba}^{\pm \mathbf{k}_{ba} \alpha} = \int_V u_b^* \epsilon_{\alpha} e^{\pm i \mathbf{k}_{ba} \mathbf{r}} \nabla u_a d^3 x$$

$$\alpha_o = \frac{e^2}{4\pi \epsilon_0 c \hbar} \quad \text{— fine structure constant in SI}$$

Note: everywhere else the fine structure constant is α

Spontaneous emission

Process in the absence of photons, i.e. when the radiation field is in the ground state. In this case $n_{\mathbf{k}\alpha} = 0$ and

$$W_{A \rightarrow B}^{\text{sp}} = \frac{e^2 h}{2m^2 \epsilon_0 V} \sum_{\mathbf{k}\alpha} \frac{1}{\omega} |M_{ba}^{-\mathbf{k}\alpha}|^2 \delta(\omega_+)$$

Plane waves in the box: $\phi_{\mathbf{k}} = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{r}}$ where

$$\mathbf{k} = \frac{2\pi}{L} \mathbf{n}; \quad \mathbf{n} = (n_1, n_2, n_3); \quad n_j = \frac{L}{2\pi} k_j, \quad j = 1, 2, 3$$

The number of photons (plane waves) in $\langle \mathbf{k}, \mathbf{k} + \Delta \mathbf{k} \rangle$:

$$\Delta n_1 \Delta n_2 \Delta n_3 = \left(\frac{L}{2\pi} \right)^3 \Delta k_1 \Delta k_2 \Delta k_3 \rightarrow \frac{V}{8\pi^3} d^3 k = k^2 dk d\Omega$$

$$\sum_{\mathbf{k}\alpha} (\dots) \Rightarrow \int_0^\infty \int_\Omega (\dots) \frac{V}{8\pi^3 c^3} \omega^2 d\omega d\Omega$$

Spontaneous emission

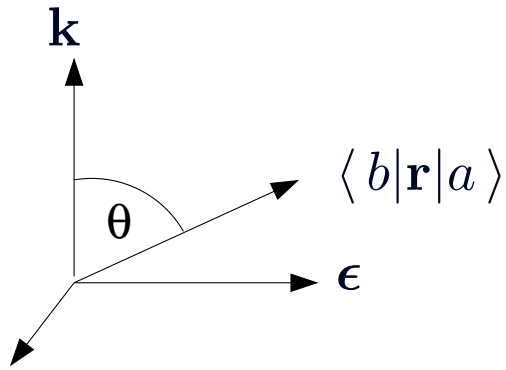
$$\begin{aligned} W_{A \rightarrow B}^{\text{sp}} &= \frac{e^2 \hbar}{8m^2 \epsilon_0 c^3 \pi^2} \int_0^\infty \int_\Omega |M_{ba}^{-\mathbf{k}\alpha}|^2 \delta(\omega_+) \omega d\omega d\Omega \\ &= \frac{\alpha_0 \hbar^2}{4\pi m^2 c^2} \int_\Omega |M_{ba}^{-\mathbf{k}_{ba}\alpha}|^2 \omega_{ba} d\Omega \end{aligned}$$

$$M_{ba}^{-\mathbf{k}_{ba}\alpha} = \int_V u_b^* \boldsymbol{\epsilon}_\alpha e^{-i\mathbf{k}_{ba}\mathbf{r}} \nabla u_a d^3x$$

Dipole approximation: $e^{-i\mathbf{k}\mathbf{r}} \Rightarrow 1$, thus

$$\int_V u_b^* \nabla u_a d^3x = \frac{m}{\hbar^2} (E_a - E_b) \int_V u_b^* \mathbf{r} u_a d^3x = \frac{m\omega_{ba}}{\hbar} \langle b|\mathbf{r}|a \rangle$$

because: $\nabla = \frac{m}{\hbar^2} \left[\mathbf{r}, \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}) \right]$, $\left(\frac{\hat{\mathbf{p}}^2}{2m} + V \right) u_a(\mathbf{r}) = E_a u_a(\mathbf{r})$



$$M_{ba}^{-\mathbf{k}_{ba}\alpha} \Rightarrow \epsilon_\alpha \langle b|\mathbf{r}|a \rangle = |\langle b|\mathbf{r}|a \rangle| \sin \theta$$

$$W_{A \rightarrow B}^{\text{sp}} = \frac{\alpha_o}{2\pi c^2} \omega_{ba}^3 |\langle b|\mathbf{r}|a \rangle|^2 \underbrace{\int_\Omega \sin \theta d\Omega}_{8\pi/3} = \frac{4\alpha_o}{3} \frac{\omega_{ba}^3}{c^2} |\langle b|\mathbf{r}|a \rangle|^2$$

DIRAC FIELD

Dirac theory versus physical reality

A basic contradiction: the one-particle interpretation of the Dirac wavefunction and the negative-energy particle sea are contradictory to each other. Two necessary conditions for the model of pair-creation to work:

- The particles (electrons) obey the Pauli principle
- The difference between the number of the positive energy electrons and positrons is conserved:

$$N(e_{E>0}^-) = N(e^-); \quad N(e_{E<0}^-) = N(e_{\text{vacuum}}^-) - N(e^+)$$
$$N(e^-) - N(e^+) = N(e_{E>0}^-) + N(e_{E<0}^-) - N(e_{\text{vacuum}}^-) = \text{const}$$

In the real world pair also boson pairs may be created (no Pauli principle) and positrons may emerge alone (not in a pair), e.g. in the beta plus decay:



CLASSICAL DIRAC FIELD

$$\begin{aligned}\mathcal{L} &= -c\hbar\bar{\psi}\gamma_{\mu}\frac{\partial\psi}{\partial x_{\mu}} - mc^2\bar{\psi}\psi \\ &= -c\hbar\bar{\psi}_{\alpha}(\gamma_{\mu})_{\alpha\beta}\frac{\partial\psi_{\beta}}{\partial x_{\mu}} - mc^2\delta_{\alpha\beta}\bar{\psi}_{\alpha}\psi_{\beta}\end{aligned}$$

$\psi_{\alpha}, \bar{\psi}_{\alpha}$ - independent field variables

$$\bar{\psi} = \psi^{\dagger}\gamma_4, \quad \text{i.e.} \quad \bar{\psi}_{\alpha} = \psi_{\beta}^{\dagger}(\gamma_4)_{\beta\alpha}$$

Variation with respect to $\bar{\psi}_{\alpha}$ leads to four Euler-Lagrange equations equivalent to the Dirac equation for ψ :

$$\frac{\partial\mathcal{L}}{\partial\bar{\psi}_{\alpha}} - \frac{\partial}{\partial x_{\mu}}\frac{\partial\mathcal{L}}{\partial\bar{\psi}_{\alpha,\mu}} = 0, \quad \alpha = 1, 2, 3, 4 \Rightarrow \gamma_{\mu}\psi_{,\mu} + \frac{mc}{\hbar}\psi = 0$$

Equation for $\bar{\psi}$

$$\frac{\partial}{\partial x_\mu} (\bar{\psi} \gamma_\mu \psi) = \frac{\partial \bar{\psi}}{\partial x_\mu} \gamma_\mu \psi + \bar{\psi} \gamma_\mu \frac{\partial \psi}{\partial x_\mu} \sim \frac{\partial j_\mu}{\partial x_\mu} = 0$$

Then, $\bar{\psi} \gamma_\mu \psi_{,\mu}$ may be replaced by $-\bar{\psi}_{,\mu} \gamma_\mu \psi$.

In effect we get:

$$\mathcal{L} = -c\hbar \bar{\psi}_{,\mu} \gamma_\mu \psi - mc^2 \bar{\psi} \psi \Rightarrow \bar{\psi}_{,\mu} \gamma_\mu - \frac{mc}{\hbar} \bar{\psi} = 0$$

Momentum density

$$\pi_\beta = \frac{\partial \mathcal{L}}{\partial \dot{\psi}_\beta} = i\hbar \bar{\psi}_\alpha (\gamma_4)_{\alpha\beta} = i\hbar \psi_\beta^\dagger$$

$$\pi = i\hbar \psi^\dagger$$

For this choice of \mathcal{L} the momentum conjugated to $\bar{\psi}_\beta$ vanishes (similarly as in the Schrödinger case)

Hamiltonian density

$$\begin{aligned}
 \mathcal{H} &= \sum_{\beta} ic\pi_{\beta} \frac{\partial \psi_{\beta}}{\partial x_4} - \mathcal{L} \\
 &= \underbrace{-c\hbar \psi^{\dagger} \psi_{,4} + c\hbar \bar{\psi} \gamma_4 \psi_{,4}}_{=0} + c\hbar \bar{\psi} \gamma_k \psi_{,k} + mc^2 \bar{\psi} \psi \\
 &= \bar{\psi} \left(c\hbar \gamma_k \frac{\partial}{\partial x_k} + mc^2 \right) \psi \\
 &= \psi^{\dagger} (-ic\hbar \boldsymbol{\alpha} \nabla + \beta mc^2) \psi
 \end{aligned}$$

$$H = \int_V \bar{\psi} \left(c\hbar \gamma_k \frac{\partial}{\partial x_k} + mc^2 \right) \psi d^3x = \int_V \psi^{\dagger} (-i\hbar c \boldsymbol{\alpha} \nabla + \beta mc^2) \psi d^3x$$

Free particle in a box

$$(c \boldsymbol{\alpha} \hat{\mathbf{p}} + \beta m c^2) \Phi_{\mathbf{k}\sigma\lambda} = \lambda E_k \Phi_{\mathbf{k}\sigma\lambda}$$

$$\mathbf{k} = \mathbf{p}/\hbar, \quad E_k = c \sqrt{k^2 \hbar^2 + m^2 c^2}, \quad \lambda = \pm 1, \quad \sigma = \boldsymbol{\sigma} \frac{\mathbf{k}}{k} = \pm \frac{1}{2}$$

Discrete, complete, and orthonormal set of plane wawewes in the box:

$$\Phi_{\mathbf{k}\sigma\lambda} = \frac{1}{\sqrt{L^3}} U_{\mathbf{k}\sigma\lambda} e^{i(\mathbf{k}\mathbf{r} - \lambda E t/\hbar)} \quad \Rightarrow \quad \psi(\mathbf{r}, t) = \sum_{\mathbf{k}\sigma\lambda} a_{\mathbf{k}\sigma\lambda} \Phi_{\mathbf{k}\sigma\lambda}(\mathbf{r}, t)$$

$$U_{\mathbf{k},+1/2,\lambda} = A \begin{bmatrix} 1 \\ 0 \\ B \\ 0 \end{bmatrix}, \quad U_{\mathbf{k},-1/2,\lambda} = A \begin{bmatrix} 0 \\ 1 \\ 0 \\ B \end{bmatrix}$$

$$A = (2\pi\hbar)^{-3/2} \sqrt{\frac{m c^2 + \lambda E_k}{2\lambda E_k}}, \quad B = \frac{c\hbar \boldsymbol{\sigma} \mathbf{k}}{m c^2 + \lambda E_k}$$

QUANTIZATION

$$a_{\mathbf{k}\sigma\lambda} \Rightarrow \hat{a}_{\mathbf{k}\sigma\lambda}$$

$$\psi(\mathbf{r}, t) \Rightarrow \hat{\psi}(\mathbf{r}, t)$$

$$\hat{\psi}(\mathbf{r}, t) = \sum_{\mathbf{k}\sigma\lambda} \hat{a}_{\mathbf{k}\sigma\lambda} \Phi_{\mathbf{k}\sigma\lambda}(\mathbf{r}, t)$$

$$\int_V \Phi_{\mathbf{k}'\sigma'\lambda'}^\dagger \Phi_{\mathbf{k}\sigma\lambda} d^3x = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \delta_{\lambda\lambda'}$$

$$\hat{H} = \int_V \hat{\psi}^\dagger (-i\hbar c \boldsymbol{\alpha} \nabla + \beta mc^2) \hat{\psi} d^3x$$

$$\{\hat{\psi}', \hat{\psi}^\dagger\} = \delta(\mathbf{r} - \mathbf{r}') \Rightarrow \{\hat{a}_{\mathbf{k}\sigma\lambda}, \hat{a}_{\mathbf{k}'\sigma'\lambda'}^\dagger\} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \delta_{\lambda\lambda'}$$

The remaining \hat{a} operators anticommute.

Hamiltonian

$$\begin{aligned}
 \hat{H} &= \int_V \hat{\psi}^\dagger (c \boldsymbol{\alpha} \mathbf{p} + \beta m c^2) \hat{\psi} d^3 x \\
 &= \sum_{\mathbf{k}\sigma\lambda} \sum_{\mathbf{k}'\sigma'\lambda'} \hat{a}_{\mathbf{k}\sigma\lambda}^\dagger \hat{a}_{\mathbf{k}'\sigma'\lambda'} \int_V \underbrace{\Phi_{\mathbf{k}\sigma\lambda}^\dagger (c \boldsymbol{\alpha} \mathbf{p} + \beta m c^2) \Phi_{\mathbf{k}'\sigma'\lambda'}}_{\lambda' E_{k'} \Phi_{\mathbf{k}'\sigma'\lambda'}} d^3 x \\
 &= \sum_{\mathbf{k}\sigma\lambda} \sum_{\mathbf{k}'\sigma'\lambda'} \lambda' E_{k'} \hat{a}_{\mathbf{k}\sigma\lambda}^\dagger \hat{a}_{\mathbf{k}'\sigma'\lambda'} \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \delta_{\lambda\lambda'} = \sum_{\mathbf{k}\sigma\lambda} \lambda E_k \hat{a}_{\mathbf{k}\sigma\lambda}^\dagger \hat{a}_{\mathbf{k}\sigma\lambda} \\
 &= \sum_{\mathbf{k}\sigma} E_k \left(\hat{a}_{\mathbf{k}\sigma+}^\dagger \hat{a}_{\mathbf{k}\sigma+} - \hat{a}_{\mathbf{k}\sigma-}^\dagger \hat{a}_{\mathbf{k}\sigma-} \right) = \sum_{\mathbf{k}\sigma} E_k (\hat{N}_{\mathbf{k}\sigma+} - \hat{N}_{\mathbf{k}\sigma-})
 \end{aligned}$$

The eigenvalues:
$$E = \sum_{\mathbf{k}\sigma} E_k \left(\underbrace{n_{\mathbf{k}\sigma+}}_{N(e_{E>0}^-)} - \underbrace{n_{\mathbf{k}\sigma-}}_{N(e_{E<0}^-)} \right)$$

Charge conjugation ($e \Rightarrow -e$) in the Dirac model

$$\left(\frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar} A_\mu \right) \gamma_\mu \psi + \frac{mc}{\hbar} \psi = 0$$

$$\left(\frac{\partial}{\partial x_\mu} + \frac{ie}{\hbar} A_\mu \right) \gamma_\mu \psi^c + \frac{mc}{\hbar} \psi^c = 0$$

$$\left(\frac{\partial}{\partial x_\mu^*} + \frac{ie}{\hbar} A_\mu^* \right) \gamma_\mu^* \psi^* + \frac{mc}{\hbar} \psi^* = 0$$

$$x_k^* = x_k, \quad x_4^* = -x_4, \quad A_k^* = x_k, \quad A_4^* = -A_4, \quad \gamma_\mu^* = (-1)^\mu \gamma_\mu$$

Let us set $\psi^c = \Gamma \psi^* \Rightarrow \Gamma = \gamma_2$ and $\psi^c = \gamma_2 \psi^*$

Charge conjugation ($e \Rightarrow -e$) in the Dirac model

$$\gamma_2 \Phi_{\mathbf{k}\sigma+}^* = \Phi_{-\mathbf{k}-\sigma-} = \Phi_{\mathbf{k}\sigma+}^c,$$

$$\gamma_2 \Phi_{-\mathbf{k}-\sigma-}^* = \Phi_{\mathbf{k}\sigma+} = \Phi_{-\mathbf{k}-\sigma-}^c$$

$E < 0$	charge	energy	momentum	spin	helicity
electrons	$- e $	$- E $	\mathbf{p}	$\frac{1}{2}\hbar\Sigma$	$\Sigma\mathbf{p}$
holes (positrons)	$+ e $	$+ E $	$-\mathbf{p}$	$-\frac{1}{2}\hbar\Sigma$	$\Sigma\mathbf{p}$

Electron and positron operators

Let us introduce new operators:

$$\hat{a}_{\mathbf{k}\sigma} = \hat{a}_{\mathbf{k}\sigma+}, \quad \hat{b}_{\mathbf{k}\sigma}^\dagger = \hat{a}_{-\mathbf{k}-\sigma-}$$

$$\hat{\psi}(\mathbf{r}, t) = \sum_{\mathbf{k}\sigma} \left(\hat{a}_{\mathbf{k}\sigma} \Phi_{\mathbf{k}\sigma+} + \hat{b}_{\mathbf{k}\sigma}^\dagger \Phi_{-\mathbf{k}-\sigma-} \right)$$

We define:

$$\Phi_{\mathbf{k}\sigma}^e \equiv \Phi_{\mathbf{k}\sigma+}, \quad \Phi_{\mathbf{k}\sigma}^p = \Phi_{-\mathbf{k}-\sigma-}$$

$\Phi_{\mathbf{k}\sigma}^e$ and $\Phi_{\mathbf{k}\sigma}^p$ are charge conjugate to each other

They correspond to the same positive energy E_k

$$\begin{aligned} \{\hat{a}_{\mathbf{k}\sigma}, \hat{a}_{\mathbf{k}'\sigma'}^\dagger\} &= \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}, & \hat{N}_{\mathbf{k}\sigma}^e &= \hat{a}_{\mathbf{k}\sigma}^\dagger \hat{a}_{\mathbf{k}\sigma} \\ \{\hat{b}_{\mathbf{k}\sigma}, \hat{b}_{\mathbf{k}'\sigma'}^\dagger\} &= \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}, & \hat{N}_{\mathbf{k}\sigma}^p &= \hat{b}_{\mathbf{k}\sigma}^\dagger \hat{b}_{\mathbf{k}\sigma} \end{aligned}$$

The remaining pairs of the new operators anticommute.

$\hat{a}_{\mathbf{k}\sigma}$ - annihilation of a particle with \mathbf{k} , σ , $\lambda = 1$

$\hat{a}_{\mathbf{k}\sigma}^\dagger$ - creation of a particle with \mathbf{k} , σ , $\lambda = 1$

$\hat{b}_{\mathbf{k}\sigma}^\dagger$ - annihilation of a particle with $-\mathbf{k}$, $-\sigma$, $\lambda = -1$
i.e. creation of a particle with $+\mathbf{k}$, $+\sigma$, $\lambda = 1$

$\hat{b}_{\mathbf{k}\sigma}$ - creation of a particle with $-\mathbf{k}$, $-\sigma$, $\lambda = -1$
i.e. annihilation of a particle with $+\mathbf{k}$, $+\sigma$, $\lambda = 1$

Hamiltonian of the electron-positron field

$$\begin{aligned}
 \hat{H} &= \sum_{\mathbf{k}\sigma} E_k \left(\hat{a}_{\mathbf{k}\sigma}^\dagger \hat{a}_{\mathbf{k}\sigma} - \hat{b}_{\mathbf{k}\sigma} \hat{b}_{\mathbf{k}\sigma}^\dagger \right) \\
 &= \sum_{\mathbf{k}\sigma} E_k \left(\hat{a}_{\mathbf{k}\sigma}^\dagger \hat{a}_{\mathbf{k}\sigma} + \hat{b}_{\mathbf{k}\sigma}^\dagger \hat{b}_{\mathbf{k}\sigma} - 1 \right) \\
 &= \sum_{\mathbf{k}\sigma} E_k \left(\hat{N}_{\mathbf{k}\sigma}^e + \hat{N}_{\mathbf{k}\sigma}^p \right) + \mathcal{E}_0
 \end{aligned}$$

$$\mathcal{E}_0 = - \sum_{\mathbf{k}\sigma} E_k \quad - \text{ a constant, infinite, "energy of the vacuum state" } |0\rangle$$

We redefine the energy scale so that $\hat{H}|0\rangle = 0$, i.e. $\hat{H} \Rightarrow \hat{H} - \mathcal{E}_0$:

$$\hat{H} = \sum_{\mathbf{k}\sigma} E_k \left(\hat{N}_{\mathbf{k}\sigma}^e + \hat{N}_{\mathbf{k}\sigma}^p \right)$$

$$E = \sum_{\mathbf{k}\sigma} E_k \left(\hat{n}_{\mathbf{k}\sigma}^e + \hat{n}_{\mathbf{k}\sigma}^p \right)$$

Note: It would be “ $-$ ” in the last equation if we had bosons

Conclusion: The requirement that the energy be positive definite leads to anticommutation relations for the Dirac field.

This means that spin $1/2$ implies Fermi-Dirac statistics.

Momentum operator:

$$\hat{\mathbf{P}} = \int_V \hat{\psi}^\dagger \hat{\mathbf{p}} \psi d^3x = \sum_{\mathbf{k}\sigma} \hbar \mathbf{k} \left(\hat{a}_{\mathbf{k}\sigma}^\dagger \hat{a}_{\mathbf{k}\sigma} + \hat{b}_{\mathbf{k}\sigma}^\dagger \hat{b}_{\mathbf{k}\sigma} \right) = \sum_{\mathbf{k}\sigma} \hbar \mathbf{k} (\hat{N}_{\mathbf{k}\sigma}^e + \hat{N}_{\mathbf{k}\sigma}^p)$$

Note: $\hat{\mathbf{p}} = -i\hbar \nabla$

Electric charge operator:

$$\hat{Q} = e \int_V \hat{\psi}^\dagger \psi d^3x = e \sum_{\mathbf{k}\sigma} \left(\hat{a}_{\mathbf{k}\sigma}^\dagger \hat{a}_{\mathbf{k}\sigma} - \hat{b}_{\mathbf{k}\sigma}^\dagger \hat{b}_{\mathbf{k}\sigma} \right) + Q_0 = \sum_{\mathbf{k}\sigma} (\hat{N}_{\mathbf{k}\sigma}^e - \hat{N}_{\mathbf{k}\sigma}^p) + Q_0$$

$$\hat{Q} \Rightarrow \hat{Q} - Q_0, \text{ i.e } \hat{\rho} = e \hat{\psi}^\dagger \psi - e \langle 0 | \hat{\psi}^\dagger \psi | 0 \rangle$$

$$[\hat{H}, \hat{Q}] = 0 \Rightarrow \text{the electric charge is conserved}$$

An alternative dealing with the infinities

\hat{H} and \hat{Q} redefined to remove the infinities:

$$\text{Let } \hat{\Psi}^\dagger \hat{\Psi} = \sum_{j=1}^4 \hat{\psi}_j^\dagger \hat{\psi}_j, \quad \hat{\tilde{\Psi}} \hat{\tilde{\Psi}}^\dagger = \sum_{j=1}^4 \hat{\psi}_j \hat{\psi}_j^\dagger \Rightarrow$$

$$\begin{aligned} \hat{H} &= \frac{1}{2} \int_V \left[\hat{\Psi}^\dagger H_D \hat{\Psi} - (\widehat{H_D \Psi}) \hat{\tilde{\Psi}}^\dagger \right] d^3x \\ &= \sum_{\mathbf{k}\sigma} E_k (\hat{N}_{\mathbf{k}\sigma}^e + \hat{N}_{\mathbf{k}\sigma}^p) = \sum_{\mathbf{k}\sigma} E_k (\hat{N}_{\mathbf{k}\sigma}^e + \hat{N}_{\mathbf{k}\sigma}^p) \end{aligned}$$

$$H_D = c\boldsymbol{\alpha}\mathbf{p} + \beta mc^2$$

$$\begin{aligned} \hat{Q} &= \frac{e}{2} \int_V \left[\hat{\Psi}^\dagger \hat{\Psi} - \hat{\tilde{\Psi}} \hat{\tilde{\Psi}}^\dagger \right] d^3x \\ &= e \sum_{\mathbf{k}\sigma} (\hat{N}_{\mathbf{k}\sigma}^e - \hat{N}_{\mathbf{k}\sigma}^p) = e \sum_{\mathbf{k}\sigma} (\hat{N}_{\mathbf{k}\sigma}^e - \hat{N}_{\mathbf{k}\sigma}^p) \end{aligned}$$

In consequence,

$$\hat{\rho} = \frac{e}{2} \left[\hat{\Psi}^\dagger \hat{\Psi} - \hat{\tilde{\Psi}} \hat{\tilde{\Psi}}^\dagger \right] = \frac{e}{2} \left[\hat{\Psi}^\dagger, \hat{\Psi} \right]$$

$$\hat{\mathbf{j}} = \frac{ce}{2} \left[\hat{\Psi}^\dagger, \boldsymbol{\alpha} \hat{\Psi} \right]$$

$$\hat{H} = \int_V \left[\hat{\Psi}^\dagger, H_D \hat{\Psi} \right]$$

Charged Klein-Gordon field:

$$\left(\square + \frac{m^2 c^2}{\hbar^2} \right) \psi = 0$$

$$\rho = \frac{i\hbar e}{2mc^2} \left(\psi^* \frac{\partial \psi}{\partial t} - \frac{\partial \psi^*}{\partial t} \psi \right)$$

$$\mathbf{j} = -\frac{i\hbar e}{2m} [\psi^* \nabla \psi - (\nabla \psi^*) \psi]$$

$$\psi_{\mathbf{k}\lambda}(\mathbf{r}, t) = A e^{i(\mathbf{k}\mathbf{r} - \lambda\omega_k t)}$$

$$\mathbf{k} = \frac{\mathbf{p}}{\hbar}, \quad \omega_k = \frac{E_k}{\hbar}, \quad E_k = c\sqrt{\hbar^2 k^2 + m^2 c^2}, \quad \lambda = \pm 1$$

$\lambda = +1$	$\lambda = -1$
$\rho_+ = \frac{e E_k}{mc^2} \psi_{\mathbf{k}+}^* \psi_{\mathbf{k}+}$	$\rho_- = -\frac{e E_k}{mc^2} \psi_{\mathbf{k}-}^* \psi_{\mathbf{k}-}$
$\psi_{\mathbf{k}+} - \text{charge } e$	$\psi_{\mathbf{k}-} - \text{charge } -e$

The Lagrange density, the Hamiltonian, quantization

$$\mathcal{L} = \frac{\partial\psi^*}{\partial t} \frac{\partial\psi}{\partial t} - c^2 (\nabla\psi^*)(\nabla\psi) - \frac{m^2 c^4}{\hbar^2} \psi^* \psi$$

$$\pi = \frac{\partial\psi^*}{\partial t}, \quad \pi^* = \frac{\partial\psi}{\partial t}$$

$$\mathcal{H} = \frac{\partial\psi^*}{\partial t} \frac{\partial\psi}{\partial t} + c^2 (\nabla\psi^*)(\nabla\psi) + \frac{m^2 c^4}{\hbar^2} \psi^* \psi$$

$$\hat{H} = \int_V \left[\frac{\partial\psi^*}{\partial t} \frac{\partial\psi}{\partial t} + c^2 (\nabla\psi^*)(\nabla\psi) - \frac{m^2 c^4}{\hbar^2} \psi^* \psi \right] d^3x$$

Particle and antiparticle operators

$$\hat{\psi} = \sqrt{\frac{\hbar}{2V}} \sum_{\mathbf{k}} \frac{1}{\sqrt{\omega_k}} \left(\hat{a}_{\mathbf{k}} e^{-i\omega_k t} + \hat{b}_{\mathbf{k}}^\dagger e^{i\omega_k t} \right) e^{i\mathbf{k}\mathbf{r}}$$

$$\begin{aligned} \hat{H} &= \sum_{\mathbf{k}} E_k \left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{b}_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger \right) \\ &= \begin{cases} \sum_{\mathbf{k}} E_k (\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} - 1), & \text{if } [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \\ \sum_{\mathbf{k}} E_k (\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} - \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} + 1), & \text{if } \{\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}^\dagger\} = \delta_{\mathbf{k}\mathbf{k}'} \end{cases} \end{aligned}$$

Conclusion: The requirement that the energy be positive definite leads to commutation relations for the Klein-Gordon field.

This means that spin 0 implies Bose-Einstein statistics.

Theorem (Pauli 1940): The fields with half-integer spin are fermionic and the fields with integer spin are bosonic.