Quantum Field Theory 1

(WS 2023/24: M. Zirnbauer)

Table of Contents

I. From Particles to Fields 3

II. Feynman Path Integral 10

III. Second Quantization 22

CHAPTER 1 : From Particles to Fields

1.1 Lagrangian Mechanics

Generalized positions $q = (q_1, q_2, \dots, q_f)$,

Generalized velocities $\dot{q} = (\dot{q}_1, \dot{q}_2, \dots, \dot{q}_f)$,

Lagrangian function $\mathcal{L}(q, \dot{q}, t)$.

Note. Initially, the positions q_i and the velocities $\dot{q}_i \equiv v_i$ are independent coordinate functions. (Thus the dot in $\dot{q}_i$ here does not mean the time derivative.)

To compute $\frac{\partial \mathcal{L}}{\partial q_i}$ and $\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \equiv \frac{\partial \mathcal{L}}{\partial v_i}$ one uses the rules $\frac{\partial \dot{q}_i}{\partial q_j} = 0 = \frac{\partial q_j}{\partial \dot{q}_i}$.

Equations of motion (Euler-Lagrange eqn):

$$\frac{\partial \mathcal{L}}{\partial q_i} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \qquad (i = 1, 2, \dots, f).$$

In this equation it is tacitly assumed that both sides are evaluated on a curve $t \mapsto \gamma(t)$ in position space:

$\frac{\partial \mathcal{L}}{\partial q_i} \equiv \frac{\partial \mathcal{L}}{\partial q_i}\left(q = \gamma(t), \dot{q} = \frac{d}{dt}\gamma(t)\right)$ and

$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \equiv \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\left(q = \gamma(t), \dot{q} = \frac{d}{dt}\gamma(t)\right)$.

These follow from a variational principle (namely, Hamilton's principle of least action):

$$0 = \delta \int_0^T dt\, \mathcal{L}(q, \dot{q}, t) = \frac{d}{ds}\bigg|_{s=0} \int_0^T dt\, \mathcal{L}(q + s\,\delta q, \dot{q} + s\,\delta\dot{q}, t)$$

$$\overset{\delta q(0) = 0 = \delta q(T)}{=} \int_0^T dt\, \delta q(t) \left(\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} \right)(t) .$$

1.2 Stable equilibrium

Consider a simple example: $\mathcal{L}(q, \dot{q}) = \frac{m}{2}|\dot{q}|^2 - U(q)$, $|\dot{q}|^2 = \sum_{i=1}^{f} \dot{q}_i^2$.

Definition. $q^{(0)}$ is called an equilibrium (position) if $(dU)_{q^{(0)}} = 0$.

Remark.

The differential dU is defined by $(dU)_q(v) := \frac{d}{ds}\Big|_{s=0} U(q + sv)$. (in affine space)

$F_q = -(dU)_q$ is called the force in q.

(Force is a co-vector, or form, <u>not</u> a vector!)

$F_q(v) = -(dU)_q(v)$ is the (negative of the) differential change of the potential energy U for a translation in the direction of v.

Definition. An equilibrium $q^{(0)}$ is called stable if $\mathrm{Hess}_{q^{(0)}}(\mathcal{U}) > 0$.

Remark. The Hessian of $\mathcal{U}$ is (in Euclidean space) the matrix of second partial derivatives: $\mathrm{Hess}_q(\mathcal{U})_{ij} = \frac{\partial^2 \mathcal{U}}{\partial q_i \partial q_j}(q)$ well-defined if $(d\mathcal{U})_q = 0$

Positivity of a matrix means that all eigenvalues are positive.

I.3 Linearization

Definition. Let $q^{(0)}$ be a stable equilibrium configuration for $\mathcal{L}(q,\dot{q}) = \frac{m}{2}|\dot{q}|^2 - \mathcal{U}(q)$. By the linearization of $\mathcal{L}$ at $q^{(0)}$ we mean the system with quadratic Lagrangian $\mathcal{L}'(u,\dot{u}) = \frac{m}{2}|\dot{u}|^2 - \frac{1}{2}\sum_{i,j}^{f}\left(\mathrm{Hess}_{q^{(0)}}(\mathcal{U})\right)_{ij} u_i u_j$.

displacements $u_j = q_j - q_j^{(0)}$

Remark. The general form of a linearization for a system with time-reversal invariance would be $\mathcal{L}'(u,\dot{u}) = \frac{1}{2}\sum_{i,j}\left(A_{ij}\dot{u}_i\dot{u}_j - B_{ij}u_i u_j\right)$ with "mass matrix" $A > 0$, and $B > 0$ for a stable equilibrium $u \equiv 0$.

Equations of motion: $\sum_j A_{ij}\ddot{u}_j = -\sum_j B_{ij}u_j \quad (i = 1, \dots, f)$.

Principal solutions $u_j(t) = e^{-i\omega t}u_j(0)$ are called normal modes.

I.4 Harmonic Chain

masses m, displacements u_j (from equilibrium)

$$\mathcal{L}(u,\dot{u}) = \frac{m}{2}\sum_{j=1}^{N}\dot{u}_j^2 - \frac{c}{2}\sum_{j=1}^{N}(u_j - u_{j-1})^2, \quad j = 1, 2, \dots, N.$$

$u_0 \equiv u_N$ (periodic boundary conditions)

L = length of chain. Instead of index j will use $x = Lj/N$ $(0 \leq x \leq L)$.

Wave number $k = \frac{2\pi}{a}\cdot\frac{j'}{N}$ $(j' = 1, \dots, N)$ is defined modulo $2\pi\mathbb{Z}/a$.

Lattice constant $a = L/N$.

Equations of motion: $m\ddot{u}_j = c\left(u_{j+1} - 2u_j + u_{j-1}\right)$.

Characteristic frequency scale: $\Omega = \sqrt{c/m}$.

Discrete Laplacian $\Delta_{jj'} = -2\delta_{jj'} + \delta_{j,j'+1} + \delta_{j,j'-1}$

e.o.m. $\ddot{u}_j = \Omega^2 (\Delta u)_j$.

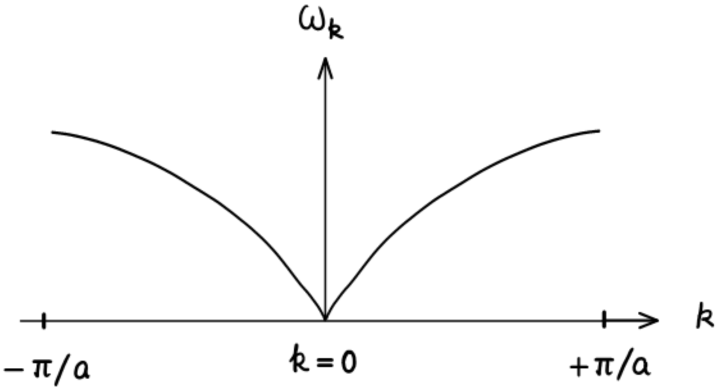
Eigenvectors of Δ: $\psi^{(k)}(x) = e^{ikx} \equiv e^{2\pi i j j'/N}$.

Eigenvalues: $(\Delta\psi^{(k)})(x) = \underbrace{\left(-2 + e^{ika} + e^{-ika}\right)}\psi^{(k)}(x)$

$$= -2 + 2\cos(ka) = -4\sin^2(ka/2) .$$

Normal modes: $\psi^{(k)}(x,t) = e^{i(kx-\omega_k t)}$

where $\omega_k = \Omega \,|\, 2\sin(ka/2) |$ (dispersion relation expressing the frequency as a function of the wave number).



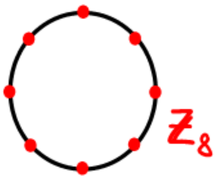
Observation. Small frequencies (or small energies) here correspond to small wave numbers or large wave lengths. Thus in the low-energy regime one expects a continuum approximation to be valid ...

I.5 Continuum approximation for the harmonic chain

Now simplified calculation by making an approximation in the Lagrangian:

Discrete model.

particle displacements: $$\mathbb{Z}_N \times \mathbb{R} \longrightarrow \mathbb{R}, \qquad (j,t) \longmapsto u_j(t).$$



↓ approximation

Continuum model.

massless scalar field $$S^1 \times \mathbb{R} \longrightarrow \mathbb{R}, \qquad (x,t) \longmapsto u(x,t).$$

Replacements $(x \longleftrightarrow j \cdot a)$.

$$u_{j+1} - u_j \longrightarrow a \frac{\partial}{\partial x} u(x,t),$$

$$\dot{u}_j \longrightarrow \frac{\partial}{\partial t} u(x,t),$$

$$\sum_{j=1}^{N} \longrightarrow \frac{1}{a} \oint_0^L dx.$$

$$S = S_{\text{disc}} = \frac{1}{2} \int_0^T dt \sum_{j=1}^{N} \left(m \dot{u}_j^2 - c\,(u_{j+1} - u_j)^2 \right)$$

$$\longrightarrow \frac{1}{2} \int_0^T dt \oint_0^L dx \left(\underbrace{\frac{m}{a} \left(\frac{\partial u}{\partial t}\right)^2 - ca \left(\frac{\partial u}{\partial x}\right)^2}_{= 2\mathcal{L}_{\text{cont}}} \right) = S_{\text{cont}}$$

Warning. Continuum approximation not unconditionally valid. Here valid for the description of the low-energy phenomenology because $\boxed{\text{small } \omega \longleftrightarrow \text{small } k}$.

Equation of motion (from Hamilton's variational principle).

$$\text{E.o.M} \rightsquigarrow \quad 0 = \delta S_{\text{cont}} = \delta \int_0^T dt \oint_0^L dx \; \mathcal{L}_{\text{cont}}\left(u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x}\right) = \dots$$

first variation $u(x,t) \longrightarrow u(x,t) + s \cdot \delta u(x,t)$

$$\dots = \frac{d}{ds}\Big|_{s=0} \int_0^T dt \oint_0^L dx \; \mathcal{L}_{\text{cont}}\left(u + s\cdot\delta u, \frac{\partial u}{\partial t} + s\frac{\partial}{\partial t}\delta u, \frac{\partial u}{\partial x} + s\frac{\partial}{\partial x}\delta u\right)$$

here

$$= \int_0^T dt \oint_0^L dx \; \delta u(x,t) \left(-\frac{m}{a}\frac{\partial^2}{\partial t^2}u + ca\frac{\partial^2}{\partial x^2}u\right) \equiv 0 \Longrightarrow$$

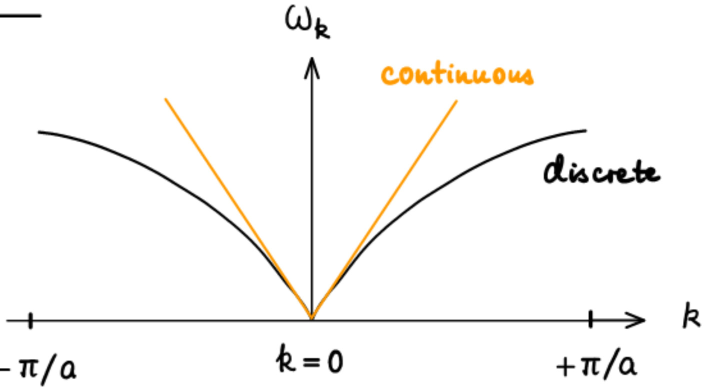
Wave equation: $\left(\frac{1}{v_s^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right)u(x,t) = 0, \qquad v_s = a\sqrt{c/m} = a\Omega.$

(Normal-mode or monochromatic) solutions $u(x,t) = e^{i(kx - \omega_k t)}$,

$$\omega_k = v_s|k| = \Omega|k|a.$$

Comparison.

	discrete	continuous
ω_k	$\Omega\lvert 2\sin(ka/2)\rvert$	$\Omega\lvert k\rvert a$



Observation: continuum approximation
OK for small wave number ($|k|a \ll 1$)
or large wave length $\sim |k|^{-1}$

Summary: here we have an instance where the following diagram is 'commutative' for the physics at long wavelengths:

$$\begin{tikzcd}
\text{Lagrangian system discrete} \arrow[r, "\text{continuum}", "\text{approximation}"'] \arrow[d, "\text{variational}"', "\text{principle}"] & \text{Lagrangian system continuous} \arrow[d, "\text{variational}"', "\text{principle}"] \\
\text{equations of motion \& solutions} \arrow[r, "\text{continuum}", "\text{approximation}"'] & \text{equations of motion \& solutions}
\end{tikzcd}$$

I.6 Legendre-Transformation

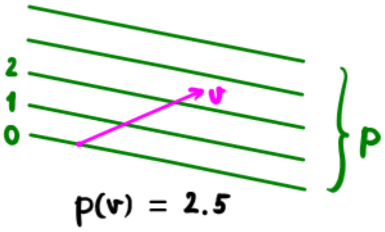
Consider a fixed configuration of all particle positions. View the Lagrangian $\mathcal{L} \equiv \mathcal{L}|_q$ as a function of the velocities $v \equiv \dot{q}$ (for the given configuration of positions q).

Thus $\mathcal{L} : V \to \mathbb{R}$ where V = vector space of velocities at q.

Assumption: $\mathcal{L}$ is convex, i.e. $\text{Hess}_v(\mathcal{L}) > 0$ for all $v \in V$. ■

The dual vector space V^* consists of all linear functions

$$p : V \to \mathbb{R}$$
$$v \mapsto p(v) = \sum p_i v^i .$$



Definition. By the canonical momentum (at q) of the Lagrangian system with Lagrangian $\mathcal{L} : V \to \mathbb{R}$ we mean the bijective map

$$\pi : V \to V^*,$$
$$v \mapsto p = (d\mathcal{L})_v .$$

In components: $p_i = \pi_i(v) = \frac{\partial \mathcal{L}}{\partial v^i}(v)$.

Inverse map: $v^i = (\pi^{-1})^i(p)$.

The Hamiltonian function $\mathcal{H} : V^* \to \mathbb{R}$ is defined by

$$\mathcal{H}(p) = \sum_i p_i (\pi^{-1})^i(p) - \mathcal{L}((\pi^{-1})(p)) .$$

Properties.

ⓘ For the inverse π^{-1} of $\pi : v \mapsto (d\mathcal{L})_v$ one has the formula $\pi^{-1} : p \mapsto (d\mathcal{H})_p$.

ⓘⓘ $\text{Hess}_v(\mathcal{L})$ and $\text{Hess}_p(\mathcal{H})$ are inverse to one another,

i.e. $V \xrightarrow{\widetilde{\text{Hess}}_v(\mathcal{L})} V^* \xrightarrow{\widetilde{\text{Hess}}_p(\mathcal{H})} V$ is the identity map

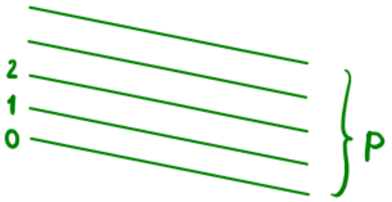
(given that $p = (d\mathcal{L})_v$).

Remarks. $\mathrm{Hess}_v(\mathcal{L}) \equiv Q : V \times V \longrightarrow \mathbb{R}$ (quadratic form) determines a linear mapping $\tilde{Q} : V \longrightarrow V^*$ by $\tilde{Q}v := Q(v,\cdot)$.

Property ⓘⓘ follows from ⓘ by differentiating $\pi^{-1} \circ \pi = \mathrm{id}$ using the chain rule.

Summary.

$$\begin{tikzcd}
\text{velocities} & & \text{momenta} \\
V \arrow[rr, shift left, "(d\mathcal{L})_v = p"] \arrow[d, "\mathcal{L} = vp - \mathcal{H}"'] & & V^* \arrow[ll, shift left, "v = (d\mathcal{H})_p"] \arrow[d, "\mathcal{H} = pv - \mathcal{L}"'] \\
\mathbb{R} & & \mathbb{R}
\end{tikzcd}$$



CHAPTER II: Feynman Path Integral

(Scene at Caltech where Professor Murray Gell-Mann is about to teach QFT)

Class: Why not use Feynman's lecture notes?

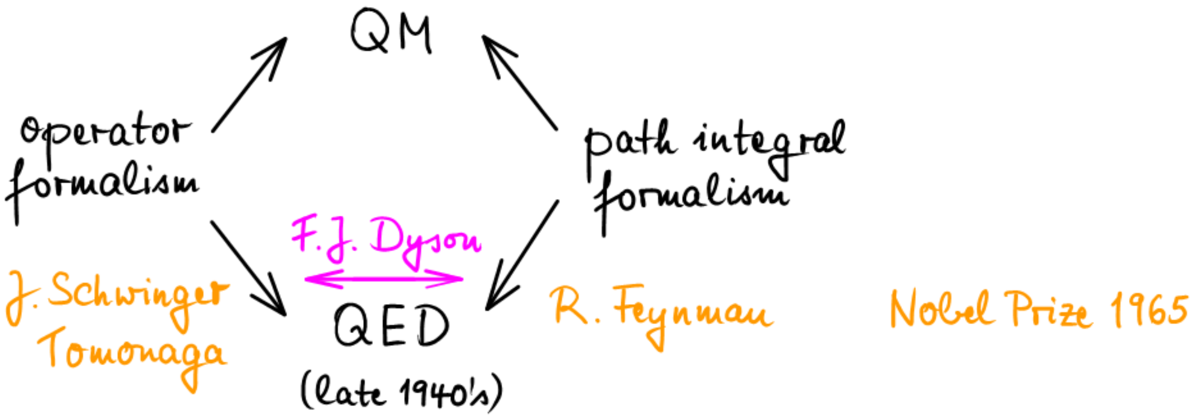
Gell-Mann: Because Feynman uses a different method than we do.

Class: What is Feynman's method?

Gell-Mann: You write down the problem. Then you look at it and you think. Then you write down the solution.

(From the Harvard QFT lecture notes of Sidney Coleman, arXiv: 1110.5013)

II.1 History / Background



Integral.

$$\overset{\text{function}}{\{x \mapsto f(x)\}} \longmapsto \int_a^b \underset{\text{measure on points}}{dx}\, f(x) \in \mathbb{R}$$

Path integral.

$$\Big\{ (\gamma : \underset{\text{path}}{t \mapsto x(t)}) \mapsto \overset{\text{functional}}{e^{iS[\gamma]/\hbar}} \Big\} \longmapsto \int \underset{\text{measure on paths}}{\mathcal{D}\gamma}\, e^{iS[\gamma]/\hbar}$$

II.2 Formulation

Quantum mechanical Hilbert space $\mathcal{V}$; Hamiltonian H (time-independent). Time evolution is a one-parameter group $t \mapsto e^{-itH/\hbar} \equiv \mathcal{U}_t$ of unitary operators on $\mathcal{V}$. Composition law: $\mathcal{U}_{t_1+t_2} = \mathcal{U}_{t_2}\mathcal{U}_{t_1}$.

For simplicity consider the Schrödinger representation for 1 particle in 1 dimension: $\mathcal{V} = L^2(\mathbb{R})$. Let $\mathbb{R} \ni x \mapsto \psi(x) \in \mathbb{C}$ denote the wave function. Time evolution then acts as an integral operator,

$$(\mathcal{U}_t\psi)(x) = \int_{\mathbb{R}} \mathcal{U}_t(x,y)\,\psi(y)\,dy = \int_{\mathbb{R}} \left(e^{-itH/\hbar}\right)(x,y)\,\psi(y)\,dy\,.$$

Dirac notation (suggestive): $\left(e^{-itH/\hbar}\right)(x,y) \equiv \left\langle x \middle| e^{-itH/\hbar} \middle| y \right\rangle$.

Composition law:

$$\left\langle x_2 \middle| e^{-i(t_2+t_1)H/\hbar} \middle| x_1 \right\rangle = \int_{\mathbb{R}} dy \left\langle x_2 \middle| e^{-it_2H/\hbar} \middle| y \right\rangle \left\langle y \middle| e^{-it_1H/\hbar} \middle| x_1 \right\rangle.$$

By iterating the composition law many times, one can reduce the calculation of $\mathcal{U}_t(x,y)$ to the calculation of the short-time propagator $\mathcal{U}_{\Delta t}(x,y)$ $\left(\Delta t = \frac{t}{N} \to 0\right)$.

Let now $H = \frac{p^2}{2m} + V(x) \equiv T + V$. With the help of the Baker–Campbell–Hausdorff formula,

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\ldots}, \quad \text{one gets} \quad e^{\varepsilon(A+B)+\mathcal{O}(\varepsilon^3)} = e^{\varepsilon B/2} e^{\varepsilon A} e^{\varepsilon B/2}$$

and hence

$$e^{-i\Delta tH/\hbar + \mathcal{O}(\Delta t^3)} = e^{-i\Delta t V/2\hbar}\, e^{-i\Delta t T/\hbar}\, e^{-i\Delta t V/2\hbar}.$$

So

$$\left\langle x \middle| e^{-i\Delta tH/\hbar} \middle| y \right\rangle = e^{-i\Delta t\left(V(x)+V(y)\right)/2\hbar} \left\langle x \middle| e^{-i\Delta t T/\hbar} \middle| y \right\rangle + \ldots$$

(with correction terms that become negligible in the limit $\Delta t \to 0$).

Now the integral kernel for the time evolution of a free particle is known exactly:

$$\left\langle x \middle| e^{-i\Delta t\, p^2/2m\hbar} \middle| y \right\rangle = \int_{\mathbb{R}} \frac{dk}{2\pi}\, e^{ik(x-y)}\, e^{-i\Delta t\,\hbar k^2/2m}$$
$$= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{1/2} e^{im(x-y)^2/2\hbar\Delta t}.$$

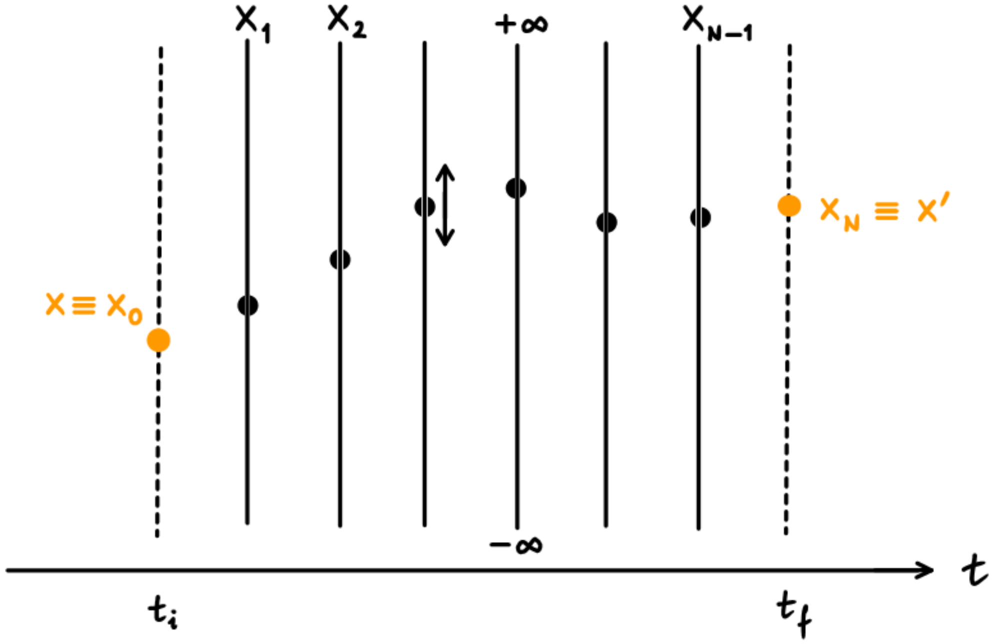
In this way, one arrives at the result

$$\langle x'|\, e^{-i(t_f-t_i)H/\hbar}\, |x\rangle = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2} \int_{\mathbb{R}} dx_1 \int_{\mathbb{R}} dx_2 \cdots \int_{\mathbb{R}} dx_{N-1}$$

$x_N \equiv x'$, $x_0 \equiv x$,

$\Delta t = \frac{t_f - t_i}{N}$.

$$\times \exp \frac{i\Delta t}{\hbar} \sum_{j=0}^{N-1} \left(\frac{m}{2} \left(\frac{x_{j+1}-x_j}{\Delta t}\right)^2 - \frac{1}{2}\left(V(x_{j+1}) + V(x_j)\right)\right).$$



In the semiclassical limit ($\hbar \to 0$) one expects the main contribution to the multiple integral to come from 'smooth' configurations $\{x_1, x_2, \dots, x_{N-1}\}$.

If so, the following approximations should be valid:

$$\Delta t \sum_{j=0}^{N-1} \left(\frac{x_{j+1}-x_j}{\Delta t}\right)^2 \longrightarrow \int_{t_i}^{t_f} dt\ \dot{x}(t)^2,$$

$$\frac{\Delta t}{2} \sum_{j=0}^{N-1} \left(V(x_{j+1}) + V(x_j)\right) \longrightarrow \int_{t_i}^{t_f} dt\ V(x(t)).$$

This leads to Feynman's formula

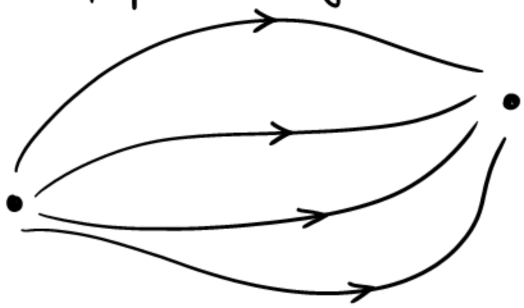
$$\langle x'|\, e^{-i(t_f-t_i)H/\hbar}\, |x\rangle = \int_{x(t_i)=x}^{x(t_f)=x'} \mathcal{D}[x(t)]\ e^{\frac{i}{\hbar}\int_{t_i}^{t_f} \mathcal{L}(x(t),\dot{x}(t))\, dt}$$

$$\mathcal{L}(x,\dot{x}) = \frac{m}{2}\dot{x}^2 - V(x)$$

for the integral kernel of the time-evolution operator as a path integral.

Remarks.

- In general, a large set of paths may make significant contributions to the path integral:



This can be seen as the path-integral manifestation of quantum interference.

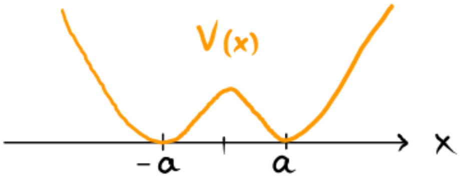
- In the semiclassical limit ($\hbar \longrightarrow 0$), the Feynman path integral can be computed by the method of stationary phase approximation. The main contribution then comes from paths $t \longmapsto \gamma(t)$ that are extrema of the action, i.e. solutions of $\delta S = 0$ or equivalently, $$0 = \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} \right) \Bigg|_{\substack{x(t) = \gamma(t) \\ \dot{x}(t) = \frac{d}{dt}\gamma(t)}} .$$

- Feynman's path-integral formula for the integral kernel of the time-evolution operator gives a perspective on Hamilton's principle of least action (viz. the boundary condition $\delta x(t_f) = 0 = \delta x(t_i)$).

II.3 Level Splitting by Quantum Tunneling

Consider the Hamiltonian $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$

of a symmetric double well potential:



The wave function of the ground state (energy E_0) is symmetric: $\psi_0(x) = \psi_0(-x)$; of the first excited state (energy E_1) it is skew: $\psi_1(x) = -\psi_1(-x)$.

Goal. Compute the level splitting $E_1 - E_0$ in the semiclassical limit ($\hbar$ small).

Trick: Consider (for large imaginary-time parameter T):

$$\langle x | e^{-TH/\hbar} | y\rangle = \psi_0(x)\, e^{-TE_0/\hbar}\, \psi_0(y) + \psi_1(x)\, e^{-TE_1/\hbar}\, \psi_1(y) + \dots$$

$$\Longrightarrow \qquad \frac{\langle a | e^{-TH/\hbar} | -a\rangle}{\langle a | e^{-TH/\hbar} | +a\rangle} = \tanh\left(\frac{T(E_1-E_0)}{2\hbar}\right) + \dots \, .$$

Method. Compute the LHS from the path integral. By inspection of the result, extract the level splitting $E_1 - E_0$.

$$\text{Recall} \quad \langle y' | e^{-iTH/\hbar} | y\rangle = \int_{x(0)=y}^{x(T)=y'} \mathcal{D}[x(t)]\ \exp\left(\frac{i}{\hbar}\int_0^T L\, dt\right).$$

Make analytic continuation from real time $T>0$ to imaginary time $-iT$.

$$dt \longrightarrow -i\,dt\,, \quad L(x,\dot{x}) \longrightarrow L(x, i\dot{x}) = -\frac{m}{2}\dot{x}^2 - V(x) = -H.$$

$$\text{Then} \quad \langle y' | e^{-TH/\hbar} | y\rangle = \int_{x(0)=y}^{x(T)=y'} \mathcal{D}[x(t)]\ \exp\left(-\frac{1}{\hbar}S_E[x]\right)$$

where $S_E = \int_0^T H\, dt = \int_0^T dt\left(\frac{m}{2}\dot{x}^2 + V(x)\right)$ "Euclidean" action functional.

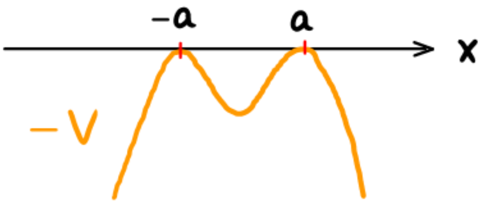
Now put $y' = a$ and $y = \mp a$ for $\frac{\text{numerator}}{\text{denominator}}$ (see above).

For small $\hbar$ the dominant contributions to the path integral come from minima of S_E, hence from solutions of the equation

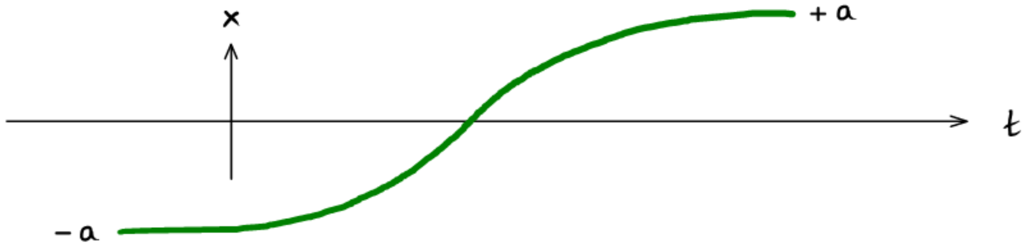
$$0 = \delta S_E \implies -m\ddot{x}(t) + V'(x(t)) = 0,$$

satisfying the boundary conditions $x(0) = \mp a$ and $x(T) = a$.

Interpretation. This is Newton's equation of motion in the inverted potential:



In the limit of an infinite imaginary-time interval, there exist special solutions such that $x(t \longrightarrow \mp\infty) = \mp a$, which are called "instantons":



Notice the conservation law (for solutions of $m\ddot{x} = +V'(x)$):

$$L = \frac{m}{2}\dot{x}(t)^2 - V(x(t)) = \text{const} \quad (\text{independent of time}).$$

Euclidean action of the instanton (const $= 0$):

$$S_E^{(0)} = \int_{-\infty}^{+\infty} dt \left(\frac{m}{2}\dot{x}^2 + V(x)\right) \overset{\frac{m}{2}\dot{x}^2 = V(x)}{=} \int_{\mathbb{R}} m\, \dot{x}(t)\, \underbrace{\dot{x}(t)\,dt}_{= dx}$$

$$= m\int_{-a}^{+a} \dot{x}(t(x))\, dx = \int_{-a}^{a} \sqrt{2mV(x)}\, dx \quad \text{since } \dot{x}(t) = \sqrt{2V(x(t))/m}.$$

Expansion of the Euclidean action functional around a critical point $t \mapsto x_0(t)$, i.e. $\delta S_E \big|_{x_0} = 0$:

$$S_E[x_0(t) + \delta x(t)] = S_E[x_0(t)] + 0 + \frac{1}{2}\int_0^T dt \int_0^T dt' \, \delta x(t) \frac{\delta^2 S_E}{\delta x(t)\, \delta x(t')}\bigg|_{t \mapsto x_0(t)} \delta x(t') + \ldots$$

$$= S_E[x_0(t)] + \frac{1}{2}(\delta x, A\, \delta x) + \ldots \quad \text{where} \quad A = -m \frac{d^2}{dt^2} + V''(x_0(t))$$

and $(\delta x, A\, \delta x) = \int_0^T dt \; \delta x(t) \, (A \, \delta x)(t)$. Note $\delta x(0) = \delta x(T) = 0$.

Recall the Gaussian integral : $\int_{\mathbb{R}} e^{-\pi x^2} dx = 1$, in several dimensions :

$$\int_{\mathbb{R}^n} e^{-\pi (x, Bx)} d^n x = \mathrm{Det}^{-1/2}(B) \quad (\text{for } \mathrm{Re}\, B > 0).$$

Path integral (a.k.a. functional integral) in Gaussian approximation :

$$\int \mathcal{D}[x(t)] \; e^{-S_E[x(t)]/\hbar} \approx e^{-S_E[x_0(t)]/\hbar} \int \mathcal{D}[\delta x(t)] \; e^{-\frac{1}{2}(\delta x, A\, \delta x)/\hbar}$$

$$\overset{?!}{=} \; e^{-S_E^{(0)}/\hbar} \; \mathrm{Det}^{-1/2}(A/2\pi\hbar) \quad \text{(needs to be defined)}.$$

We can be cavalier about this as we want a ratio (of determinants).

In the case of $\langle a | e^{-TH/\hbar} | a \rangle$ the dominant contribution comes from the trivial solution $x(t) = a = \text{const}$.

Let $A_0 \equiv -m \frac{d^2}{dt^2} + V''(a)$, $A_1 \equiv -m \frac{d^2}{dt^2} + V''(x_0(t))$ (instanton).

$$\text{Then} \quad \frac{\langle a | e^{-TH/\hbar} | -a \rangle}{\langle a | e^{-TH/\hbar} | +a \rangle} \approx \frac{\mathrm{Det}^{1/2}(A_0)}{\mathrm{Det}^{1/2}(A_1)} \, e^{-S_E^{(0)}/\hbar}.$$

Warning: there is a problem lurking here, as A_1 develops a zero mode in the limit of large T.

Instanton calculus for the level splitting of a symmetric double well:

$$\frac{\langle a|e^{-TH/\hbar}|-a\rangle}{\langle a|e^{-TH/\hbar}|a\rangle} = \tanh\left(\frac{T(E_1-E_0)}{2\hbar}\right) = \frac{\sum_{n\ \text{odd}}\left(T(E_1-E_0)/2\hbar\right)^n/n!}{\sum_{n\ \text{even}}\left(T(E_1-E_0)/2\hbar\right)^n/n!}$$

$$\approx \frac{"n=1"}{"n=0"} = \frac{T}{2\hbar}(E_1-E_0) \underset{\nearrow\ \text{ratio of imaginary-time path integrals}}{\overset{\text{one-instanton approximation}}{=}} e^{-S_E^{(0)}/\hbar}\,\mathrm{Det}^{-1/2}(A_1/A_0)\ ?$$

Let us now explain what the problem is: appearance of a zero mode in A_1.

Qualitative discussion of zero mode.

We differentiate the Euler–Lagrange equation $-m\ddot{x}_0(t) + V'(x_0(t)) = 0$ with respect to t to obtain $\left(-m\frac{d^2}{dt^2} + V''(x_0(t))\right)\dot{x}_0(t) = 0$.

For $x_0(t) = \text{const}$ this is not informative, as $\dot{x}_0(t)$ is then the zero function. However, in the case of the instanton $x_0(t)$ we learn that the fluctuation operator A_1 annihilates the function $\dot{x}_0(t) \neq 0$.

For finite T this zero mode does not satisfy Dirichlet boundary conditions, as $\dot{x}_0(t=0) \neq 0$. Yet, $\dot{x}_0(t=0) \longrightarrow 0$ as $T \longrightarrow \infty$.

Heuristic picture. The instanton has "finite width" as a function of time (hence its name, which derives from "instant(aneous)"). For a finite time interval T the action functional $S_E[x(t)]$ with boundary conditions $x(0) = -a$ and $x(T) = a$ has a unique minimum; that's the instanton with center at the midpoint $t = T/2$. However, in the limit of infinite T the uniqueness of the minimum gets lost; the center of the instanton can then be shifted away from $T/2$ without changing the value of S_E (which is what gives rise to the zero mode).

The variable position of the instanton is called a "soft mode" (for T large but finite). It is not correct to assume that one may treat fluctuations around the instanton in Gaussian approximation for the soft mode / zero mode. Rather one must give special treatment to the zero mode by integrating over all possible positions of the instanton — this yields a factor of $\int_0^T dt = T$.

The Gaussian approximation is fine for all modes but the zero modes.

Thus the cure for our problem is to replace $\mathrm{Det}^{-1/2}(A_1/A_0) \longrightarrow \mathrm{Det}^{-1/2}(\tilde{A}_1/A_0)\int_0^T dt$ where $\mathrm{Det}^{-1/2}(\tilde{A}_1)$ is $\mathrm{Det}^{-1/2}(A_1)$ with the zero mode omitted.

II.4 Fluctuation Determinant

Motivation. Determinants of (differential) operators are ubiquitous in quantum field theory. Here are two reasons why:

ⓘ Any Lagrangian at the fundamental level is quadratic in the fermion fields. By integrating over the fermions one obtains a determinant.

ⓘⓘ The so-called one-loop effective action (to be introduced later) is (the logarithm of a) determinant.

So, we'll spend some time and effort learning how to compute determinants. Here we begin with the simple 1D case of the Gaussian-fluctuation determinant for our instanton path. ■

By standardization of the time interval $[0,T] \to [0,1]$ and scaling of the operator $\text{const}\cdot A \to A$, consider from now on the standard operator

$$A = -\frac{d^2}{dt^2} + W(t)$$

on the unit interval $t \in [0,1]$ with Dirichlet boundary conditions.

A good quantity to consider is the ratio of functional determinants (see above)

$$\frac{\mathrm{Det}(A_0)}{\mathrm{Det}(A_1)} \quad \text{for} \quad A_1 = -\frac{d^2}{dt^2} + W(t) > 0$$
$$\text{and } A_0 = -\frac{d^2}{dt^2} + \text{const} > 0 .$$

In fact, if $\lambda_n(A_j)$ are the eigenvalues of A_j, then

$$\frac{\mathrm{Det}(A_0)}{\mathrm{Det}(A_1)} := \lim_{N\to\infty} \prod_{n=1}^{N} \frac{\lambda_n(A_0)}{\lambda_n(A_1)} \quad \text{converges (for bounded } W).$$

Lemma. Let ψ_j be a solution of the differential equation $A_j\psi_j = 0$ with initial data $\psi_j(0) = 0$ and $\psi_j'(0) = 1$ $(j = 0, 1)$. Then

$$\frac{\mathrm{Det}(A_1)}{\mathrm{Det}(A_0)} = \frac{\psi_1(1)}{\psi_0(1)} .$$

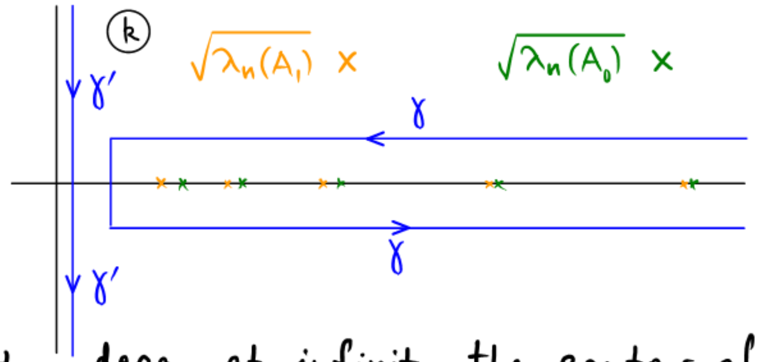
Proof (Kirsten & McKane, math-ph/0305010).

An operator A with a sequence of eigenvalues $0 < \lambda_1 < \lambda_2 < \ldots < \lambda_n < \ldots$ of quadratic growth determines a ζ-function $\zeta_A(s) = \sum_{n=1}^{\infty} \lambda_n^{-s}$ for $\mathrm{Re}(s) > 1/2$. Due to cancellations, $\zeta_{A_1}(s) - \zeta_{A_0}(s) = \sum_{n=1}^{\infty}\left(\lambda_n(A_1)^{-s} - \lambda_n(A_0)^{-s}\right)$ exists for $\mathrm{Re}(s) > -\varepsilon$, and one has $\zeta'_{A_1}(0) - \zeta'_{A_0}(0) = -\sum_{n=1}^{\infty}\left(\ln\lambda_n(A_1) - \ln\lambda_n(A_0)\right)$.

Hence, $\exp\left(\zeta'_{A_1}(0) - \zeta'_{A_0}(0)\right) = \dfrac{\mathrm{Det}(A_0)}{\mathrm{Det}(A_1)}$.

Now write the difference of ζ-functions as a contour integral. For this, define $\psi_{j,k}(t)$ (for $j = 0, 1$) by $(A_j - k^2)\,\psi_{j,k}(t) = 0$; $\psi_{j,k}(0) = 0$, $\psi'_{j,k}(0) = 1$. The function $k \mapsto \psi_{j,k}(1)$ hits zero whenever k^2 hits an eigenvalue of A_j. Thus we get the following integral representation:

$\zeta_{A_1}(s) - \zeta_{A_0}(s) = \dfrac{1}{2\pi i}\displaystyle\int_{k\in\gamma} k^{-2s}\, d\ln\frac{\psi_{1,k}(1)}{\psi_{0,k}(1)}$, for the choice of integration contour γ shown in this figure:



Because the integrand has sufficient decay at infinity, the contour of integration can be deformed to $\gamma' = i\mathbb{R} + \varepsilon$ (with the negative orientation). Putting $k = r\,e^{i\varphi}$ $(r > 0)$ we get $k^{-2s} = r^{-2s}\,e^{-is\pi}$ along the positive imaginary axis and $k^{-2s} = r^{-2s}\,e^{+is\pi}$ along the negative one. By using $\psi_{j,ir} = \psi_{j,-ir}$ and $(e^{is\pi} - e^{-is\pi})/2i = \sin(\pi s)$ we can combine the contributions from the two half-axes. Thus $\zeta_{A_1}(s) - \zeta_{A_0}(s) =$
$= \dfrac{\sin(\pi s)}{\pi}\displaystyle\int_0^{\infty} r^{-2s}\, d\ln\frac{\psi_{1,ir}(1)}{\psi_{0,ir}(1)}$. Differentiation at $s = 0$ gives

$$\zeta'_{A_1}(0) - \zeta'_{A_0}(0) = \int_0^{\infty} d\ln\frac{\psi_{1,ir}(1)}{\psi_{0,ir}(1)} = -\ln\frac{\psi_{1,0}(1)}{\psi_{0,0}(1)} = -\ln\frac{\psi_1(1)}{\psi_0(1)}.$$

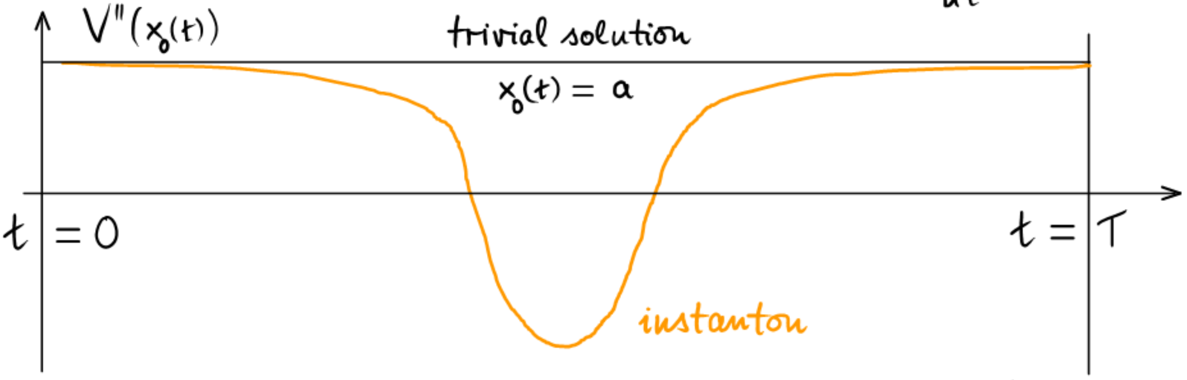
By exponentiating this relation we arrive at the desired result ■

Remark. Thus the problem of calculating the ratio of determinants has been reduced to the problem of solving an ordinary differential equation.

Application: level splitting for symmetric double well potential.

Recall $S_E = \int_0^T dt \left(\frac{m}{2} \dot{x}^2 + V(x) \right)$, $A_1 = - m \frac{d^2}{dt^2} + V''(x_0(t))$,

$$A_0 = - m \frac{d^2}{dt^2} + V''(a) .$$



From the Lemma (above) we know that $\mathrm{Det}^{-1/2}(A_1/A_0) = \left(\frac{\psi_1(1)}{\psi_0(1)} \right)^{-1/2}$,

where $\left(- \frac{d^2}{d\tau^2} + \frac{T^2}{m} V''(a) \right) \psi_0(\tau) = 0$, $\psi_0(0) = 0$, $\dot{\psi}_0(0) = 1$,

$$\left(- \frac{d^2}{d\tau^2} + \frac{T^2}{m} V''(x_0(\tau T)) \right) \psi_1(\tau) = 0, \quad \psi_1(0) = 0, \quad \dot{\psi}_1(0) = 1.$$

One immediately sees that $\psi_0(\tau) = \beta^{-1} \sinh(\beta\tau)$, $\beta = \sqrt{\frac{T^2}{m} V''(a)}$.

Hence $\psi_0(1) = \frac{\sinh(\beta)}{\beta} \underset{T \text{ large}}{\approx} \frac{e^\beta}{2\beta}$.

Complication for A_1 : zero/soft mode (see earlier and also below).

Summary. $\tanh\left(\frac{T}{2\hbar}(E_1 - E_0) \right) \overset{T \text{ large}}{=} \frac{\langle a | e^{-TH/\hbar} | -a \rangle}{\langle a | e^{-TH/\hbar} | +a \rangle} =$

$$= \int_{x(0)=-a}^{x(T)=a} \mathcal{D}[x(t)] \, e^{-S_E[x(t)]/\hbar} \Bigg/ \int_{x(0)=+a}^{x(T)=a} \mathcal{D}[x(t)] \, e^{-S_E[x(t)]/\hbar}$$

$$= \frac{1\text{-}\mathcal{I}. + 3\text{-}\mathcal{I}. + 5\text{-}\mathcal{I}. + \cdots}{0\text{-}\mathcal{I}. + 2\text{-}\mathcal{I}. + 4\text{-}\mathcal{I}. + \cdots} = \ldots$$ (dilute instanton gas approximation)

$$\ldots = \frac{\sum_{q=0}^{\infty} e^{-(2q+1) S_E^{(0)}/\hbar} \mathrm{Det}^{-1/2}(\tilde{A}_{2q+1}) T^{2q+1}/(2q+1)!}{\sum_{q=0}^{\infty} e^{-2q S_E^{(0)}/\hbar} \mathrm{Det}^{-1/2}(\tilde{A}_{2q}) T^{2q}/(2q)!}$$

$$= \tanh\left(e^{-S_E^{(0)}/\hbar} \omega T \right) \Longrightarrow E_1 - E_0 = 2\hbar\omega \, e^{-S_E^{(0)}/\hbar} .$$

Uses $\int\limits_{0 < t_1 < t_2 < \cdots < t_n < T} dt_1 dt_2 \cdots dt_n = T^n/n!$ and $\mathrm{Det}^{-1/2}(\tilde{A}_n)/\mathrm{Det}^{-1/2}(A_0) = \omega$

Computation of $\mathrm{Det}(\tilde{A}_1)$ (following Kirsten & McKane).

Recall $\zeta_A(s) = (2\pi i)^{-1} \int_\gamma k^{-2s}\, d \ln \psi_k(1)$ where

$$(A - k^2)\psi_k(t) = 0, \quad \psi_k(0) = 0, \quad \dot{\psi}_k(0) = 1.$$

We wish to modify this so as to omit the zeromode (if present).
In the presence of a zero mode $\psi_k(1)$ vanishes as k^2 for $k^2 \to 0$.
Therefore, let $f_k \overset{\mathrm{def}}{=} -\psi_k(1)/k^2$.

An expression for f_k in terms of known quantities can be produced as follows.
Let $\tau \longmapsto u_0(\tau)$ denote the zero mode: $A u_0 = 0$, $u_0(0) = u_0(1) = 0$.

Then $$k^2 \langle u_0, \psi_k \rangle \equiv k^2 \int_0^1 d\tau\, u_0(\tau)\psi_k(\tau) = \int_0^1 d\tau\, u_0(\tau)\, A\, \psi_k(\tau)$$

$$= \int_0^1 d\tau \left(u_0(\tau) A \psi_k(\tau) - \psi_k(\tau) A u_0(\tau) \right) = \int_0^1 d\tau \frac{d}{d\tau}\left(-u_0(\tau)\frac{d}{d\tau}\psi_k(\tau) + \psi_k(\tau)\frac{d}{d\tau}u_0(\tau) \right)$$

$$= \left(-u_0(\tau)\frac{d}{d\tau}\psi_k(\tau) + \psi_k(\tau)\frac{d}{d\tau}u_0(\tau) \right)\Bigg|_{\tau=0}^{\tau=1} = \psi_k(1)\, \dot{u}_0(1).$$

Hence $$f_k = -\psi_k(1)/k^2 = -\frac{\langle u_0, \psi_k \rangle}{\dot{u}_0(1)}.$$

Consider now the integral $\frac{1}{2\pi i} \int_\gamma k^{-2s}\, d \ln\left((1-k^2) f_k \right)$ with the same contour γ as before. The function $k \longmapsto (1-k^2) f_k$ has the same large-k behavior as $\psi_k(1)$. It has the same zeroes as $\psi_k(1)$ but for the missing zero eigenvalue $k^2 = 0$ and an extra eigenvalue $k^2 = 1$; the latter, however, contributes a residue independent of s. Therefore, the integral above gives the correct (derivative of the) ζ-function: $\zeta'_{\hat{A}}(s) = \frac{1}{2\pi i} \frac{d}{ds} \int_\gamma k^{-2s}\, d \ln\left((1-k^2) f_k \right)$.
By proceeding in the same way as before (deform the contour, etc.) one obtains the result

$$\zeta'_{\hat{A}}(0) = -\ln f_0 + \text{const}, \quad \text{and} \quad \mathrm{Det}(\tilde{A}) = \exp\left(-\zeta'_{\hat{A}}(0) \right) \propto f_0 = -\frac{\langle u_0, \psi_0 \rangle}{\dot{u}_0(1)}.$$

III. Second Quantization

= formalism for the quantum mechanics of many particles / fields

fermions / matter vs. bosons / radiation

Wavefunctions are totally skew totally symmetric

HERE: emphasize the universal algebraic structures!

III.1 Harmonic oscillator algebra (review)

Hamiltonian $H = \frac{p^2}{2m} + \frac{m}{2}\omega^2 q^2$, oscillator length $\ell = \sqrt{\frac{\hbar}{m\omega}}$.

Introduce $a = \frac{1}{\sqrt{2}}\left(\frac{q}{\ell} + i\,\frac{\ell p}{\hbar}\right)$, $a^+ = \frac{1}{\sqrt{2}}\left(\frac{q}{\ell} - i\,\frac{\ell p}{\hbar}\right)$.

Commutator: $[a, a^+] = 1$, $H = \hbar\omega\left(a^+a + \frac{1}{2}\right)$.

The operator a^+a has spectrum $\mathbb{N} \cup \{0\}$. Reason:

$[a^+a, a^+] = +a^+$, $[a^+a, a] = -a$ and $a\,|0\rangle = 0$,

so $a^+a\,(a^+)^n|0\rangle = (a^+)^n|0\rangle\, n$. ground state

Take-away messages.

$$\text{Hilbert space} = |0\rangle\cdot\mathbb{C} \oplus a^+|0\rangle\cdot\mathbb{C} \oplus (a^+)^2|0\rangle\cdot\mathbb{C} \oplus \ldots \oplus (a^+)^n|0\rangle\cdot\mathbb{C} \oplus \ldots$$

$$= \bigoplus_{n=0}^{\infty} \mathcal{F}^n, \quad \mathcal{F}^n = (a^+)^n|0\rangle\cdot\mathbb{C}.$$

Raising operators $a^+ : \mathcal{F}^n \longrightarrow \mathcal{F}^{n+1}$ create one oscillator quantum.

Lowering operators $a : \mathcal{F}^n \longrightarrow \mathcal{F}^{n-1}$ annihilate one oscillator quantum.

III.2 Symmetric algebra & Weyl algebra

Generalization to N-dimensional harmonic oscillator:

$$[a_i, a_j] = 0 = [a_i^+, a_j^+], \quad [a_i, a_j^+] = \delta_{ij}.$$

$$\mathcal{F}^0 = |0\rangle \cdot \mathbb{C}, \quad \mathcal{F}^1 = \mathrm{span}_{\mathbb{C}}\{a_i^+|0\rangle\}, \ldots, \quad \mathcal{F}^n = \mathrm{span}_{\mathbb{C}}\{a_{i_1}^+ a_{i_2}^+ \cdots a_{i_n}^+|0\rangle\}.$$

Universal math allows re-interpretation:

oscillator quanta $\longrightarrow$ particles (bosons).

Wave functions for identical bosons are totally symmetric under particle exchange. This motivates the following definition.

Definition. Let V be a complex vector space. The symmetric algebra $S(V)$ is the associative algebra generated by $V \oplus \mathbb{C}$ with relations $vv' - v'v = 0$ (for all $v, v' \in V$).

Remark 1. "associative algebra generated by $V \oplus \mathbb{C}$" means that the algebra elements are polynomials in vectors from V with complex coefficients.

Remark 2. The symmetric algebra comes with a $\mathbb{Z}$-grading $S(V) = \bigoplus_{n=0}^{\infty} S^n(V)$ by the degree of the polynomial: $S^0(V) = \mathbb{C}$, $S^1(V) = V$, $S^2(V) = V \otimes_{sym} V$.
The physical meaning of the degree is boson number.

Translation to physics notation. For this, V needs to be a complex Hilbert space (carrying a Hermitian scalar product). Let $\{e_i\}$ be an orthonormal basis of V. Then

math		phys
$S^0(V) = \mathbb{C} \ni 1$	$\longleftrightarrow$	$\|0\rangle$
$S^1(V) = V \ni e_i$	$\longleftrightarrow$	$a_i^+\|0\rangle$
$S^2(V) \ni e_i e_j = e_j e_i$	$\longleftrightarrow$	$a_i^+ a_j^+\|0\rangle = a_j^+ a_i^+\|0\rangle$

Exercise. $\dim S^n(\mathbb{C}^N) = \binom{N+n-1}{n}$.

Definition. Let V be a complex vector space. The **Weyl algebra** $W(V \oplus V^*)$ is the associative algebra generated by $V \oplus V^* \oplus \mathbb{C}$ with relations

$$vv' - v'v = 0, \quad \varphi\varphi' - \varphi'\varphi = 0, \quad \varphi v - v\varphi = \varphi(v) \cdot 1$$

$$(\text{for all } v, v' \in V \text{ and } \varphi, \varphi' \in V^*).$$

Outlook. $v \in V$ will give the creation operators
and $\varphi \in V^*$ the annihilation operators.

Remark. Hermann Weyl $\neq$ André Weil.

Operations on $S(V)$.

i. **Symmetric multiplication** $\mu(v) : S^n(V) \longrightarrow S^{n+1}(V) \quad (v \in V)$

$$\Phi \longmapsto v\Phi = \Phi v .$$

ii. **Derivation** $\delta(\varphi) : S^n(V) \longrightarrow S^{n-1}(V) \quad (\varphi \in V^*)$

defined by $\delta(\varphi) \cdot 1 = 0, \quad \delta(\varphi) \cdot v = \varphi(v) \in \mathbb{C},$

$\delta(\varphi) \cdot (vv') = \varphi(v)\, v' + \varphi(v')\, v$ & continue by Leibniz product rule.

Note $\delta(\varphi) \cdot v^n = n\, v^{n-1} \varphi(v)$.

Physics notation. Orthonormal basis $\{e_i\}$ of V, $\{f^i\}$ of V^*.
Then $\mu(e_i) \equiv a_i^+$, $\delta(f^i) \equiv a_i$ and $a_i |0\rangle = 0$, $a_i a_j^+ |0\rangle = |0\rangle\, \delta_{ij}$,

$$a_i a_j^+ a_k^+ |0\rangle = a_i^+ |0\rangle\, \delta_{jk} + a_j^+ |0\rangle\, \delta_{ik} \quad \text{etc.}$$

Fact. The Weyl algebra $W(V \oplus V^*)$ is represented on the symmetric algebra $S(V)$ by $V \ni v \longmapsto \mu(v)$ and $V^* \ni \varphi \longmapsto \delta(\varphi)$.

Proof left as an exercise.

III.3 Tutorial on Hermitian conjugation

Canonical adjoint.

Let L be a linear transformation between two vector spaces X and Y, $L: X \longrightarrow Y$. Then L has a canonical adjoint (or transpose) $L^t: Y^* \longrightarrow X^*$ defined by $(L^t\varphi)(x) = \varphi(Lx)$ (for all $x \in X$ and $\varphi \in Y^*$).

Fréchét-Riesz isomorphism.

Let V be a Hermitian vector space, i.e. a complex vector space carrying a Hermitian scalar product $\langle \cdot , \cdot \rangle_V : V \times V \longrightarrow \mathbb{C}$.

Then one has an isomorphism (FR) $c_V : V \longrightarrow V^*$, $v \longmapsto \langle v, \cdot \rangle_V$.

Note that c_V is complex antilinear: $c_V \lambda = \bar{\lambda} c_V$ where $\bar{\lambda}$ is the complex conjugate of $\lambda \in \mathbb{C}$.

In physics c_V is called the Dirac ket-to-bra bijection $|v\rangle \longmapsto \langle v|$.

Hermitian conjugation.

Let $L : X \longrightarrow Y$ be a linear transformation between two Hermitian vector spaces X and Y. Then L has a Hermitian adjoint $L^\dagger : Y \longrightarrow X$ defined by $L^\dagger = c_X^{-1} \circ L^t \circ c_Y$. In the form of a diagram,

$$\begin{tikzcd}
X \arrow[r, "L"] \arrow[d, "c_X"'] & Y \arrow[d, "c_Y"] \arrow[l, bend left=60, "L^\dagger"] \\
X^* & Y^* \arrow[l, "L^t"]
\end{tikzcd}$$

Exercise: $\langle Lx, y \rangle_Y = \langle x, L^\dagger y \rangle_X$ (for all $x \in X$ and $y \in Y$).

III.4 Hermitian structure of bosonic Fock space

Invariant formulation.

Recall: single-particle Hilbert space $V \curvearrowright$ bosonic Fock space $S(V)$.

Now the Hermitian scalar product on V induces a Hermitian scalar product on $S(V) \equiv \mathcal{F}$ as follows.

Decompose $\mathcal{F} = \bigoplus_{n \geq 0} \mathcal{F}^n$, $\mathcal{F}^n = S^n(V)$, by the degree (or boson number).

Take the Hermitian scalar product on $\mathcal{F}$ to be diagonal in n, i.e. states with different boson number are orthogonal to each other. For fixed n, let $\Phi, \Phi' \in S^n(V)$ be two pure elements, i.e.

$$\Phi = v_1 v_2 \cdots v_n \quad \text{and} \quad \Phi' = v_1' v_2' \cdots v_n' \quad \text{for any } v_i, v_i' \in V.$$

Then define the Hermitian scalar product of Φ and Φ' as a sum over permutations:

$$\langle \Phi, \Phi' \rangle_{\mathcal{F}^n} = \sum_{\pi \in S_n} \langle v_1, v'_{\pi(1)} \rangle_V \langle v_2, v'_{\pi(2)} \rangle_V \cdots \langle v_n, v'_{\pi(n)} \rangle_V .$$

This definition is extended to general elements $\Phi, \Phi' \in S^n(V)$ by complex linearity in the right argument and antilinearity in the left argument of the Hermitian scalar product.

Note the special case: $\langle v^n, v^n \rangle_{\mathcal{F}^n} = n! \, \langle v, v \rangle_V^n$.

Physics notation.

Orthonormal basis $\{e_i\}$ of V.

$$1 \equiv |0\rangle, \quad e_i \equiv a_i^+ |0\rangle, \quad e_i e_j \equiv a_i^+ a_j^+ |0\rangle, \quad \text{etc.}$$

Let $\Phi = a^+_{i_1} a^+_{i_2} \cdots a^+_{i_n} |0\rangle$ and $\Phi' = a^+_{i_1'} a^+_{i_2'} \cdots a^+_{i_n'} |0\rangle$. Then

$$\langle \Phi | \Phi' \rangle = \langle 0 | a_{i_n} \cdots a_{i_2} a_{i_1} a^+_{i_1'} a^+_{i_2'} \cdots a^+_{i_n'} |0\rangle = \sum_{\pi \in S_n} \delta_{i_1 i'_{\pi(1)}} \, \delta_{i_2 i'_{\pi(2)}} \cdots \delta_{i_n i'_{\pi(n)}} .$$

Exercise.

$$\begin{tikzcd} S^n(V) \arrow[r, shift left, "\mu(v)"] & S^{n+1}(V) \arrow[l, shift left, "\mu(v)^+ = \delta(cv)"] \end{tikzcd} , \qquad \begin{tikzcd} S^n(V) \arrow[r, shift left, "\delta(\varphi)"] & S^{n-1}(V) \arrow[l, shift left, "\delta(\varphi)^+ = \mu(c^{-1}\varphi)"] \end{tikzcd} .$$

III.5 Second quantization of one-body operators

Single-particle Hilbert space V.

How does an operator L given on V (position, momentum, energy, etc.) become an operator $\hat{L}$ acting on the bosonic Fock space $\mathcal{F} = S(V)$?

Physics notation. As usual, fix some orthonormal basis $|i\rangle$ (Dirac).

Then $1 = \sum_i |i\rangle\langle i|$ and $L = \sum_{ij} |i\rangle\langle i|L|j\rangle\langle j|$

$$\text{and } \hat{L} = \sum_{ij} a_i^+ \langle i|L|j\rangle a_j = \sum_{ij} \langle i|L|j\rangle a_i^+ a_j \, .$$

Math picture.

$1_V = \sum_i e_i \otimes f^i$ (for any basis e_i of V, with f^i the dual basis of V^*).

Check: $1_V \cdot v = \sum_i e_i \, f^i(v) = \sum_i v^i e_i = v$ ✓

Now $L = \sum_i (Le_i) \otimes f^i$. Expanding $Le_i = \sum_j e_j L^j{}_i$ view this as a polynomial $\sum_{ij} L^j{}_i \, e_j f^i$ in the Weyl algebra for $V \oplus V^*$ and second-quantize by $e_j \longrightarrow \mu(e_j)$ and $f^i \longrightarrow \delta(f^i)$. Hence $\hat{L} = \sum_{ij} L^j{}_i \, \mu(e_j)\, \delta(f^i)$.

Fact. Second quantization $L \longrightarrow \hat{L}$ preserves the commutator:

$$[\hat{L}, \hat{M}] = \widehat{[L,M]} \, .$$

Proof. $\hat{L} = \sum_i \mu(Le_i)\, \delta(f^i)$, $\hat{M} = \sum_j \mu(Me_j)\, \delta(f^j)$.

Multiply & subtract:
$$[\hat{L}, \hat{M}] = \sum_{ij} \mu(Le_i)\, \delta(f^i)\, \mu(Me_j)\, \delta(f^j) - \sum_{ij} \mu(Me_j)\, \delta(f^j)\, \mu(Le_i)\, \delta(f^i) \, .$$

Move the high-lighted derivations past the symmetric multiplication operators μ on their right. The resulting terms cancel by $\mu(v)\mu(v') = \mu(v')\mu(v)$ and $\delta(\varphi)\,\delta(\varphi') = \delta(\varphi')\,\delta(\varphi)$. What remains are the commutator terms $[\delta(\varphi), \mu(v)] = \sum_i \varphi_i v^i \cdot 1_{S(V)}$ due to moving δ past μ. Hence,

$$[\hat{L}, \hat{M}] = \sum_{ij} \mu(Le_i)\, f^i(Me_j)\, \delta(f^j) - \sum_{ij} \mu(Me_j)\, f^j(Le_i)\, \delta(f^i) \, .$$

By using that $f^i(Me_j) = M^i{}_j$ and $\sum_i \mu(Le_i)\, M^i{}_j = \mu\left(L \sum e_i M^i{}_j\right) = \mu\left(LMe_j\right)$

$$[\hat{L}, \hat{M}] = \sum_j \mu(LMe_j)\, \delta(f^j) - \sum_i \mu(MLe_i)\, \delta(f^i)$$
$$= \sum_i \mu([L,M]e_i)\, \delta(f^i) = \widehat{[L,M]} \, .$$

III.6 Canonical Quantization (bosons)

We have learned about second quantization for bosonic particles, where the single-particle Hilbert is given a priori by the particle picture. What to do in situations such as those of electromagnetic waves or vibrational excitations of solids where particle-like objects (photons resp. phonons) emerge due to quantization but are not present in the initial setting from the classical theory?

Canonical quantization is a constructive procedure by which to handle such situations. Its basic setting is that of a classical phase space (spanned by positions and momenta). For simplicity we here assume the phase space, W, to be a (real) vector space. (In the more general setting of a manifold W we would be drawn into the realm of geometric quantization.) Two structures are needed on W for canonical quantization:

1. Symplectic structure α.

This is a skew-symmetric (and non-degenerate) bilinear form $\alpha : W \times W \longrightarrow \mathbb{R}$, (On a manifold W, α would be a closed 2-form.) $\alpha(u,v) = -\alpha(v,u)$.

Example. $\dim_{\mathbb{R}} W = 2$. $\left.\begin{array}{r} \text{position } q : W \longrightarrow \mathbb{R} \\ \text{momentum } p : W \longrightarrow \mathbb{R} \end{array}\right\}$ local coordinates with differentials dq and dp.

Here $\alpha = dp \wedge dq$ (the exterior product $\wedge$ will be formally introduced later).

Vector fields ∂_q and ∂_p defined by

$$dq(\partial_q) = 1 = dp(\partial_p),$$
$$dq(\partial_p) = 0 = dp(\partial_q).$$

HERE $(W = \mathbb{R}^2)$: $\partial_q \equiv e_q$, $\partial_p \equiv e_p$ (constant).

Then
$$\alpha(e_p, e_q) = 1 = -\alpha(e_q, e_p),$$
$$\alpha(e_p, e_p) = 0 = \alpha(e_q, e_q).$$

2. Complex structure J.

This is a linear transformation $J: W \longrightarrow W$ (in the setting of a manifold W, the complex structure would be a tensor field $J \in \Gamma(W, \mathrm{End}(TW))$) with the property $J^2 = -1$.

The complex structure is required to be compatible with the symplectic structure:

$$\alpha(w, w') = \alpha(Jw, Jw') \text{ for all } w, w' \in W.$$

Note that a symmetric bilinear form $g : W \times W \longrightarrow \mathbb{R}$ is defined by $g(w,w') = \alpha(w, Jw')$. Indeed, $g(w,w') = \alpha(Jw, J^2 w') = \alpha(w', Jw) = g(w', w)$.

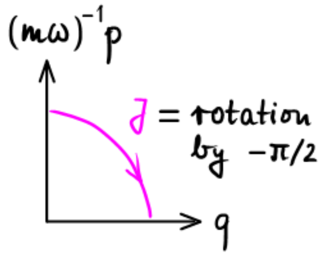
Postulate: $g(w,w) \geqslant 0$. If so, the positive function g ("energy") defines a Euclidean metric structure on the phase space W.

Example. $W = \mathrm{span}\{e_q, e_p\} \cong \mathbb{R}^2$.

Define J by $Je_q = -m\omega\, e_p$, $Je_p = +(m\omega)^{-1} e_q$.

J acts on $q, p \in W^*$ by J^{-1t}: $J \cdot q = J^{-1t} q = -(m\omega)^{-1} p$,

$J \cdot p = J^{-1t} p = +m\omega\, q$.



$g(e_q, e_q) = m\omega$, $g(e_p, e_p) = (m\omega)^{-1}$, so $\frac{\omega}{2} g = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2$.

Remark.

$$\begin{tikzcd} W & W \arrow[l, "J^{-1}"'] \\ W^* \arrow[r, "J^{-1t}"'] & W^* \end{tikzcd}$$

Perspective / Outlook (on canonical quantization).

Symplectic structure α → Heisenberg commutation relations for q, p;

Complex structure J → Fock vacuum (ground state);

α & J → Hermitian structure of Fock space.

Lagrangian subspaces.

A linear transformation $J: W \longrightarrow W$, $J^2 = -1$, must have eigenvalues $\pm i$, and therefore cannot be diagonalized over $\mathbb{R}$. Pass to the complexification $W_{\mathbb{C}} = W \otimes \mathbb{C}$. Extend α and J to $W_{\mathbb{C}}$ by complex linearity.

Make eigenspace decomposition: $W \otimes \mathbb{C} = V \oplus \tilde{V} = E_{-i}(J) \oplus E_{+i}(J)$.

Explicitly: $V = \{ w + iJw \mid w \in W \}$ and $\tilde{V} = \{ w - iJw \mid w \in W \}$.

Note the isomorphisms (over $\mathbb{R}$)

$$\left.\begin{array}{ll} W \longrightarrow V, & w \longmapsto w + iJw \\ W \longrightarrow \tilde{V}, & w \longmapsto w - iJw \end{array}\right\} \Longrightarrow \dim V = \dim \tilde{V}.$$

The compatibility of J with the skew-symmetric bilinear form α has the consequence that the subspaces V and $\tilde{V}$ of $W_{\mathbb{C}}$ are Lagrangian:
$\forall v, v' \in V$: $\alpha(v, v') = \alpha(Jv, Jv') = i^2 \alpha(v, v') = 0$ and the same for $\alpha|_{\tilde{V}}$.

Now the non-degenerate bilinear form α determines a canonical isomorphism $W_{\mathbb{C}} \longrightarrow W_{\mathbb{C}}^*$ by $w \longmapsto \alpha(w, \cdot)$. We can make this isomorphism dimensionless by scaling with Planck's constant: $I: W_{\mathbb{C}} \longrightarrow W_{\mathbb{C}}^*$, $w \longmapsto \frac{i}{\hbar} \alpha(w, \cdot)$.
By the Lagrangian property of the subspaces $V \subset W_{\mathbb{C}}$ and $\tilde{V} \subset W_{\mathbb{C}}$, we have the restrictions $I(V) = \tilde{V}^*$ and $I(\tilde{V}) = V^*$. [Equivalently, we say that there is a pairing $V \otimes \tilde{V} \longrightarrow \mathbb{C}$, i.e. V and $\tilde{V}$ are dual to each other.]

Hermitian structure.

The Lagrangian subspace $V \subset W \otimes \mathbb{C}$ carries a Hermitian scalar product

$$h: V \times V \longrightarrow \mathbb{C} \text{ by } h(v, v') = h(w + iJw, w' + iJw') \overset{\text{def}}{=} -\frac{i}{\hbar} \alpha(w - iJw, w' + iJw').$$

Indeed,

$$\overline{h(v, v')} = +\frac{i}{\hbar} \alpha(w + iJw, w' - iJw') = -\frac{i}{\hbar} \alpha(w' - iJw', w + iJw) = h(v', v)$$

and $h(v, v) = -\frac{i}{\hbar} \alpha(w - iJw, w + iJw) = \frac{2}{\hbar} \alpha(w, Jw) = \frac{2}{\hbar} g(w, w) \geq 0$.

Notice $\operatorname{Re} h(v, v') = \frac{2}{\hbar} g(w, w')$ and $\operatorname{Im} h(v, v') = -\frac{2}{\hbar} \alpha(w, w')$.

Example/Exercise.

Suppose we didn't know how to quantize a single bosonic degree of freedom (say, 1D harmonic oscilator). Then we could turn to canonical quantization:

Let $W = \mathrm{span}\{e_q, e_p\} \cong \mathbb{R}^2$,

$\alpha(e_p, e_q) = 1 = -\alpha(e_q, e_p)$, $\alpha(e_p, e_p) = 0 = \alpha(e_q, e_q)$,

and $J e_q = -m\omega\, e_p$, $J e_p = +(m\omega)^{-1} e_q$.

1. Verify that $V = E_{-i}(J) = \mathbb{C}\cdot v^+$ for

$$v^+ = \frac{\ell}{\sqrt{2}}\left(e_q - i\, m\omega\, e_p\right), \qquad \ell = \sqrt{\frac{\hbar}{m\omega}}.$$

2. Adopting the isomorphism $\mathcal{I}: W_{\mathbb{C}} \longrightarrow W_{\mathbb{C}}^*$,

$$w \longmapsto \frac{i}{\hbar}\alpha(w, \cdot),$$

show that $\mathcal{I}(e_q) = -\frac{i}{\hbar} p$ and $\mathcal{I}(e_p) = \frac{i}{\hbar} q$.

[Equivalently, one has $\mathcal{I}^{-1^t}(p) = \frac{\hbar}{i} e_q$ and $\mathcal{I}^{-1^t}(q) = i\hbar e_p$.]

3. Deduce that $\mathcal{I}(v^+) = a^+ = \frac{1}{\sqrt{2}}\left(\frac{1}{\ell} q - \frac{i\ell}{\hbar} p\right)$.

Remark.	V	$V \longrightarrow \mathrm{End}\, S(V)$	$V \equiv S^1(V) \subset S(V)$
math	e_i	$e_i \longmapsto \mu(e_i)$	$e_i = \mu(e_i)\cdot 1$
phys	e_i	$e_i \longmapsto a_i^+$	$e_i = a_i^+ \lvert 0\rangle$

$\longleftarrow - - - - - - - - \longrightarrow$

not be confused!

Summary: canonical quantization for bosons.

A triple (W, α, J) (as introduced in the previous lecture) determines a "polarization" $W_{\mathbb{C}} = E_{-i}(J) \oplus E_{+i}(J) \equiv V \oplus \tilde{V}$ by the eigenspaces of J. It also determines a Hermitian scalar product (let $v = w + iJw$, $v' = w' + iJw'$) by $\langle v, v'\rangle_V = \frac{2}{\hbar}\left(g(w,w') - i\alpha(w,w')\right)$.

The Hilbert space of the canonically quantized theory is the Fock space $S(V)$.

NEW. By the isomorphism $\tilde{V}^* \cong I(V)$, linear functions $\varphi \in W^*$ (such as position $q: W \longrightarrow \mathbb{R}$ and momentum $p: W \longrightarrow \mathbb{R}$) become operators on $S(V)$ as $W_{\mathbb{C}}^* = V^* \oplus \tilde{V}^* \cong V^* \oplus I(V) \ni \varphi + I(v) \longmapsto \delta(\varphi) + \mu(v)$.

Example: 1D harmonic oscillator.

Take J = phase flow by $T_{osc}/4$ $\left(T_{osc} = \frac{2\pi}{\omega}\right)$. Then

$$V = E_{-i}(J) = \mathbb{C}\cdot(e_q + iJe_q) = \mathbb{C}\cdot(e_q - im\omega e_p) = \mathbb{C}\cdot\left(e_q - i\frac{\hbar}{\ell^2}e_p\right)$$

and $V^* \ni \frac{1}{\sqrt{2}}\left(\frac{q}{\ell} + i\ell\frac{p}{\hbar}\right) \equiv \underset{\text{unit co-vector}}{\varphi} \longmapsto \delta(\varphi) \equiv a$. Similarly,

$$\tilde{V}^* = I(V) \ni \frac{1}{\sqrt{2}}\left(\frac{q}{\ell} - i\ell\frac{p}{\hbar}\right) = I(v) \longmapsto \mu(v) \equiv a^+.$$

So, $p = \frac{1}{\sqrt{2}}\frac{\hbar}{i\ell}(a - a^+) = p_{V^*} + p_{I(V)} \in V^* \oplus I(V)$.

[Note the arbitrary phase convention: $a\,e^{-i\theta}$, $a^+ e^{i\theta}$ would do just as well!]

Question: what is $\hat{J}$?

Answer: $\hat{J} = e^{-i(T_{osc}/4)\hat{H}/\hbar} = e^{-i\frac{\pi}{2}a^+a}\cdot e^{-i\pi/4}$.

Exercise. $\hat{J}a^+\hat{J}^{-1} = -i a^+$, $\hat{J}a\hat{J}^{-1} = +ia$.

III.7 Canonical quantization of scalar field

Recall the continuum approximation to the harmonic chain (Chapter 1). $\rightsquigarrow$ massless scalar bosonic field ($\approx$ displacement field) in (1+1) space-time dimensions $u : [0,L] \times \mathbb{R} \longrightarrow \mathbb{R}$,

$$(x,t) \longmapsto u(x,t).$$

Adopt Dirichlet boundary conditions: $u(0,t) = 0 = u(L,t)$.

Recall the Lagrangian density function: $\mathcal{L} = \frac{m}{2}\left(\frac{\partial u}{\partial t}\right)^2 - \frac{\varkappa}{2}\left(\frac{\partial u}{\partial x}\right)^2$. The classical equation of motion ($\rightsquigarrow$ Euler-Lagrange) is the wave equation: $\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right) u(x,t) = 0$, $\quad c = \sqrt{\varkappa/m}$.

We now proceed to specify the triple (W, α, J).

1. The classical phase space here is the vector space W of solutions of the classical equation of motion. (Note $\dim W = \infty$.) That space W of solutions,

$$u(x,t) = \sum_{n=1}^{\infty} \sin(k_n x)\left(Q_n \cos(\omega_n t) + P_n \sin(\omega_n t)\right)$$

where $k_n = n\pi/L$ and $\omega_n = n\pi c/L$,

is parametrized by pairs of real numbers $\{Q_n, P_n\}_{n=1}^{\infty}$.

2. The symplectic structure $\alpha : W \times W \longrightarrow \mathbb{R}$ is given by

$$\alpha(u,v) = m \int_0^L dx \left(v(x,t)\frac{\partial}{\partial t}u(x,t) - u(x,t)\frac{\partial}{\partial t}v(x,t)\right).$$

Note that $\alpha(u,v)$ is time-independent (and hence a well-defined real number). Indeed,

$$\frac{\partial}{\partial t}\alpha(u,v) = m\int_0^L dx\left(v\frac{\partial^2}{\partial t^2}u - u\frac{\partial^2}{\partial t^2}v\right) = mc^2\int_0^L dx\left(v\frac{\partial^2}{\partial x^2}u - u\frac{\partial^2}{\partial x^2}v\right)$$

$$= \varkappa\int_0^L dx\,\frac{\partial}{\partial x}\left(v\frac{\partial}{\partial x}u - u\frac{\partial}{\partial x}v\right) = \varkappa\left(v\frac{\partial}{\partial x}u - u\frac{\partial}{\partial x}v\right)\Big|_{x=0}^{x=L} = 0.$$

The explicit expression for α in terms of the coefficients Q_n, P_n is

$$\alpha(u,u') = \sqrt{m\varkappa}\sum_{n=1}^{\infty} n\pi\,\tfrac{1}{2}\left(P_n Q_n' - Q_n P_n'\right).$$

3. The complex structure $J: W \longrightarrow W$ is the classical phase flow by one quarter period $T_n/4 = \pi/2\omega_n$ for each normal mode.

Use $\cos(\theta+\pi/2) = -\sin\theta$, $\sin(\theta+\pi/2) = \cos\theta$ to find

$$(Ju)(x,t) = \sum_{n=1}^{\infty}\sin(k_n x)\Big(P_n\cos(\omega_n t) - Q_n\sin(\omega_n t)\Big).$$

Thus $J\cdot(Q_n, P_n) = (P_n, -Q_n)$. Clearly, $J^2 = -1$.

One easily sees that $\alpha(u,v) = \alpha(Ju, Jv)$, and the associated quadratic form $g(u) = \alpha(u, Ju) = \sqrt{m\varkappa}\sum_{n=1}^{\infty}\frac{n\pi}{2}\left(Q_n^2 + P_n^2\right)$ is positive. ✓

4. We construct the polarization $W_{\mathbb{C}} = E_{-i}(J) \oplus E_{+i}(J)$.

$$\pm i\,(Q_n, P_n) = J\cdot(Q_n, P_n) = (P_n, -Q_n) \implies P_n = \pm i Q_n.$$

Hence a solution $u^+ \in E_{-i}(J) \equiv V$ is of the form

$$u^+(x,t) = \sum_{n=1}^{\infty} C_n \sin(k_n x)\, e^{-i\omega_n t} \qquad (\text{"positive-energy soln"}),$$

while for $u^- \in E_{+i}(J) \equiv \tilde{V} \cong V^*$ we have

$$u^-(x,t) = \sum_{n=1}^{\infty} D_n \sin(k_n x)\, e^{+i\omega_n t} \qquad (\text{"negative-energy solution"}).$$

General case: $u(x,t) = \sum_{n=1}^{\infty}\sin(k_n x)\left(A_n e^{-i\omega_n t} + \bar{A}_n e^{+i\omega_n t}\right)$

$$= u^+(x,t) + u^-(x,t), \quad A_n = \tfrac{1}{2}(Q_n + iP_n), \quad \bar{A}_n = \tfrac{1}{2}(Q_n - iP_n).$$

We are now in a position to set up the Fock–Hilbert space and quantize the field [$\longrightarrow$ next lecture].

Tutorial. In a vector space V with basis $\{e_i\}$, vectors $v \in V$ are expressed as sums $\sum_i e_i v^i$ with coefficients v^i. The latter are promoted to linear coordinate functions x^i on V by setting $x^i(v) := v^i$. In the same way, having fixed a basis for W by $\{\sin(k_n x)\cos(\omega_n t), \sin(k_n x)\sin(\omega_n t)\}_{n=1}^{\infty}$, we promote the coefficients Q_n, P_n to linear functions $Q_n, P_n : W \longrightarrow \mathbb{R}$ (without any change of notation). Viewed as functions on the classical phase space W, the $Q_n, P_n \in W^*$ are akin to positions and momenta.

5. Field quantization.

As usual, the Hilbert space is the bosonic Fock space $S(V)$.

ⓐ The coefficients $A_n = \frac{1}{2}(Q_n + iP_n) \in V^*$ (as linear functions $V \to \mathbb{C}$) quantize as annihilation operators, $A_n \longmapsto \delta(A_n)$.

ⓑ The complex conjugated coefficients $\bar{A}_n = \frac{1}{2}(Q_n - iP_n) \in \tilde{V}^*$ quantize as creation operators, $\bar{A}_n \longmapsto \mu(\mathcal{I}^{-1}(\bar{A}_n))$, where the inverse of the isomorphism $\mathcal{I} : V \to \tilde{V}^*$, $v \longmapsto \frac{i}{\hbar}\alpha(v, \cdot)$ comes into play.

6. Commutation relations.

The annihilation operators $\delta(A_n)$ commute amongst themselves, and so do the creation operators $\mu(\mathcal{I}^{-1}(\bar{A}_n))$. To determine the nonvanishing commutator of $\delta(A_n)$ with $\mu(\mathcal{I}^{-1}(\bar{A}_n))$, we need to work out the inverse image $\mathcal{I}^{-1}(\bar{A}_n)$ for $\mathcal{I}$.

Reexpressing the symplectic structure α in terms of the $A_n, \bar{A}_n$ we find

$$\alpha = \sqrt{m\varkappa} \sum_{n=1}^{\infty} \frac{n\pi}{i} \left(A_n \bar{A}_n' - \bar{A}_n A_n' \right).$$

Let $E_n \in V$, $\bar{E}_n \in \tilde{V}$ be the basis vectors dual to A_n, $\bar{A}_n$ (in particular, $A_n(E_n) = 1$). Then

$$\mathcal{I}(E_n) = \frac{i}{\hbar}\,\alpha(E_n, \cdot) = \sqrt{m\varkappa}\,\frac{n\pi}{\hbar}\,\bar{A}_n \quad \text{and}$$

$$\mathcal{I}^{-1}(\bar{A}_n) = \frac{\hbar E_n}{n\pi\sqrt{m\varkappa}} . \quad \text{Hence,}$$

$$\left[\delta(A_n), \mu(\mathcal{I}^{-1}(\bar{A}_n))\right] = A_n\big((\mathcal{I}^{-1}(\bar{A}_n))\big)\,\underline{1} = \frac{\hbar A_n(E_n)}{n\pi\sqrt{m\varkappa}}\,\underline{1} = \frac{\hbar\cdot 1}{Lm\omega_n} .$$

7. Calibration & mode expansion of field

Let $u_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x)$, so that $\int_0^L dx\, u_n^2(x) = 1$. Define calibrated mode operators a_n, a_n^+ by

$$\delta(A_n) = \sqrt{\frac{\hbar}{Lm\omega_n}}\,a_n , \quad \mu(\mathcal{I}^{-1}(\bar{A}_n)) = \sqrt{\frac{\hbar}{Lm\omega_n}}\,a_n^+ .$$

Then we have the following mode expansion for the quantized field u:

$$\hat{u}(x,t) = \sum_{n=1}^{\infty} u_n(x)\sqrt{\frac{\hbar}{2m\omega_n}}\left(a_n e^{-i\omega_n t} + a_n^+ e^{+i\omega_n t}\right),$$

$$[a_{n'}, a_n^+] = \delta_{n'n} , \quad [a_{n'}, a_n] = 0 = [a_{n'}^+, a_n^+] .$$

8. Quantum Hamiltonian & zero-point energy

$$\frac{\partial}{\partial t}\hat{u}(x,t) = \sum_{n=1}^{\infty} u_n(x)\sqrt{\frac{\hbar\omega_n}{2m}}\,\frac{1}{i}\left(a_n e^{-i\omega_n t} - a_n^+ e^{+i\omega_n t}\right),$$

$$\frac{\partial}{\partial x}\hat{u}(x,t) = \sum_{n=1}^{\infty}\sqrt{\frac{2}{L}}\cos(k_n x)\,k_n\sqrt{\frac{\hbar}{2m\omega_n}}\left(a_n e^{-i\omega_n t} + a_n^+ e^{+i\omega_n t}\right),$$

$$\leadsto \hat{H} = \int_0^L dx\left(\frac{m}{2}\left(\frac{\partial\hat{u}}{\partial t}\right)^2 + \frac{\varkappa}{2}\left(\frac{\partial\hat{u}}{\partial x}\right)^2\right)$$

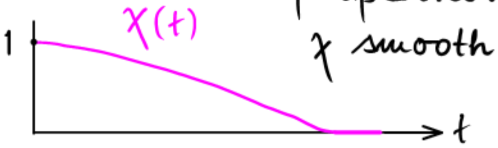
$$= \sum_{n=1}^{\infty}\frac{\hbar\omega_n}{4}\left(\left(\frac{1}{i}a_n e^{-i\omega_n t} - \frac{1}{i}a_n^+ e^{+i\omega_n t}\right)^2 + \left(a_n e^{-i\omega_n t} + a_n^+ e^{+i\omega_n t}\right)^2\right)$$

$$= \sum_{n=1}^{\infty}\frac{\hbar\omega_n}{2}\left(a_n a_n^+ + a_n^+ a_n\right) = \sum_{n=1}^{\infty}\hbar\omega_n\left(a_n^+ a_n + \frac{1}{2}\right).$$

Ground state $a_n|0\rangle = 0$. Zero-point energy $= \sum_{n=1}^{\infty}\hbar\omega_n/2 = \infty$??

III.8 Casimir effect

cutoff function:



properties: $\chi(0) = 1$, $\chi'(0) \leqslant 0$,
χ smooth and compactly supported.

Regularized vacuum energy $E_{reg}(a) = \frac{\hbar c}{2} \sum_{n=1}^{\infty} \frac{n\pi}{L} \chi\left(\frac{n\pi}{L} a\right)$.
cutoff length a ($a \to 0$).

CLAIM. E_{reg} has a Laurent expansion

$$E_{reg}(a) = \sum_{j \geqslant -1} E_j a^{2j} = E_{-1} a^{-2} + E_0 + E_1 a^2 + \dots$$

with universal finite part $E_0 = -\frac{\hbar c \pi}{24 L}$.

Remark. Casimir force $= \frac{\hbar c \pi}{24} \left(-\frac{dL}{L^2}\right)$ (1D scalar bosonic field).

Poisson summation formula. Let $f \in L^1(\mathbb{R})$ with Fourier transform $\tilde{f}(k) = \int_{\mathbb{R}} f(x) e^{ikx} dx$. Then $\sum_{n \in \mathbb{Z}} f(n) = \sum_{m \in \mathbb{Z}} \tilde{f}(2\pi m)$ if the right-hand side exists.

Remark. Example of strong coupling — weak coupling duality.

Verification.

$$\sum_{n \in \mathbb{Z}} f(n) = \int_{\mathbb{R}} dx\, f(x) \sum_{n \in \mathbb{Z}} \delta(x-n)$$

$$= \int_{\mathbb{R}} dx\, f(x) \sum_{m \in \mathbb{Z}} e^{2\pi i m x} = \sum_{m \in \mathbb{Z}} \tilde{f}(2\pi m).$$

Adapt this to our situation: $\varepsilon = \pi a / L$ ($\varepsilon \to 0+$). Compute

$$\sum_{n=1}^{\infty} n \chi(\varepsilon n) = \int_0^{\infty} dt \sum_{n \in \mathbb{Z}} \delta(t-n)\, t\, \chi(\varepsilon t) = \sum_{m \in \mathbb{Z}} \int_0^{\infty} dt\, e^{2\pi i m t} t \chi(\varepsilon t)$$

$$= \int_0^{\infty} dt\, t \chi(\varepsilon t) + 2 \sum_{m=1}^{\infty} \int_0^{\infty} dt \cos(2\pi m t)\, t \chi(\varepsilon t)$$

$$= \varepsilon^{-2} \int_0^{\infty} dt\, t \chi(t) + \frac{1}{\pi} \sum_{m=1}^{\infty} \frac{d}{dm} \underbrace{\int_0^{\infty} dt \sin(2\pi m t)\, \chi(\varepsilon t)}$$

$$\overset{\text{p.I.}}{=} \frac{\chi(0)}{2\pi m} + \frac{\varepsilon}{2\pi m} \int_0^{\infty} dt \cos(2\pi m t)\, \chi'(\varepsilon t).$$

Hence,

$$E_{reg}(a) = \frac{\hbar c}{2} \sum_{n=1}^{\infty} \frac{n\pi}{L} \chi\left(\frac{n\pi}{L} a\right) = E_{-1} a^{-2} + E_0 + E_1 a^2 + \dots$$

$$E_{-1} = \frac{\hbar c L}{2\pi} \int_0^{\infty} t \chi(t)\, dt \text{ (non-universal)}, \quad E_0 = -\frac{\hbar c}{4\pi L} \sum_{m=1}^{\infty} \frac{1}{m^2} = -\frac{\hbar c \pi}{24 L} \blacksquare$$

III.9 Bogoliubov Transformations (bosons)

$$\begin{tikzcd} & \text{(for) particles } \checkmark \\ \text{Second quantization} \arrow[ur, bend left] \arrow[dr, bend right] & \\ & \text{canonical quantization } \checkmark \text{ (for waves, fields)} \end{tikzcd}$$

$$\begin{tikzcd} \text{"Physical" particle (observable)} \arrow[r, phantom, "\overset{\text{in general}}{\neq}"] & \text{"bare" particle (Lagrangian)} \arrow[l, bend left, "\text{Bogoliubov} - \text{T.}"] \end{tikzcd}$$

Example: harmonic chain (start from discrete setting).

$$H = \sum_{n \in \mathbb{Z}} \left(\frac{p_n^2}{2m} + \frac{c}{2} (q_n - q_{n+1})^2 \right) \qquad 2c = m\omega_0^2$$

$$= \sum_{n \in \mathbb{Z}} \left(\frac{p_n^2}{2m} + \frac{m}{2}\omega_0^2 q_n^2 \right) - \frac{m}{2}\omega_0^2 \sum_{n \in \mathbb{Z}} q_n q_{n+1} .$$

Introduce oscillators (as the "bare particles"): $q_n = \frac{\ell}{\sqrt{2}}(a_n + a_n^+)$,

$$p_n = \frac{\hbar}{\sqrt{2} i \ell}(a_n - a_n^+), \qquad \ell = \sqrt{\frac{\hbar}{m\omega_0}} .$$

$$\rightsquigarrow\ H = \frac{\hbar\omega_0}{2} \sum_n (a_n^+ a_n + a_n a_n^+) - \frac{\hbar\omega_0}{4} \sum_n (a_n + a_n^+)(a_{n+1} + a_{n+1}^+) .$$

Note: by the presence of $a_n^+ a_{n+1}^+ + a_n a_{n+1}$ the number of oscillator quanta ("bare" particles) is not conserved!

Goal. Construct linear combinations β_k of the a_n, a_n^+ so as to diagonalize the Hamiltonian: $H = \sum_k \epsilon_k \beta_k^+ \beta_k + \underbrace{\text{const}}_{= E_0 = \text{ground-state energy}}$

Step 1. Fourier transform $\rightsquigarrow$ momentum representation:

$$\left. \begin{aligned} a_n &= \int_{-\pi}^{+\pi} \frac{dk}{2\pi} e^{-ikn} b_k \\ a_n^+ &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{ikn} b_k^+ \end{aligned} \right\} \quad [b_{k'}, b_k^+] = 2\pi\,\delta(k - k') .$$

Use $\sum_{n\in\mathbb{Z}} e^{ikn} = 2\pi\,\delta(k)$, $\quad k\in[-\pi,\pi]$. Then

$$H = \frac{\hbar\omega_0}{2}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\Big(\big(1-\tfrac{1}{2}\cos k\big)\big(b_k^+b_k + b_{-k}b_{-k}^+\big) - \tfrac{1}{2}\cos k\,\big(b_k^+b_{-k}^+ + b_{-k}b_k\big)\Big)$$

$$= \frac{\hbar\omega_0}{2}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\begin{pmatrix} b_k^+ & b_{-k}\end{pmatrix}\begin{pmatrix} 1-\frac{1}{2}\cos k & -\frac{1}{2}\cos k \\ -\frac{1}{2}\cos k & 1-\frac{1}{2}\cos k\end{pmatrix}\begin{pmatrix} b_k \\ b_{-k}^+\end{pmatrix}$$

$$= \frac{\hbar\omega_0}{2}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\begin{pmatrix} b_k^+ & -b_{-k}\end{pmatrix}\begin{pmatrix} 1-\frac{1}{2}\cos k & -\frac{1}{2}\cos k \\ +\frac{1}{2}\cos k & -(1-\frac{1}{2}\cos k)\end{pmatrix}\begin{pmatrix} b_k \\ b_{-k}^+\end{pmatrix}.$$

Note: while the last modification makes the 2×2 matrix non-Hermitian, this is a characteristic and actually crucial feature; cf. below.

Matrix diagonalization: $\begin{pmatrix} 1-\frac{1}{2}\cos k & -\frac{1}{2}\cos k \\ +\frac{1}{2}\cos k & -(1-\frac{1}{2}\cos k)\end{pmatrix} = \begin{pmatrix} u_k & v_k \\ v_k & u_k\end{pmatrix}\begin{pmatrix} \epsilon_k & 0 \\ 0 & -\epsilon_k\end{pmatrix}\begin{pmatrix} u_k & v_k \\ v_k & u_k\end{pmatrix}^{-1}.$

Bogoliubov transformation: $\begin{pmatrix} \beta_k^+ & -\beta_{-k}\end{pmatrix} = \begin{pmatrix} b_k^+ & -b_{-k}\end{pmatrix}\begin{pmatrix} u_k & v_k \\ v_k & u_k\end{pmatrix}$;

u_k, v_k even and real functions of k, $\;u_k^2 - v_k^2 = 1\;$ (for $[b_{k'}, b_k^+] = [\beta_{k'}, \beta_k^+]$).

Note $\begin{pmatrix} u_k & v_k \\ v_k & u_k\end{pmatrix}^{-1}\begin{pmatrix} b_k \\ b_{-k}^+\end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ -v_k & u_k\end{pmatrix}\begin{pmatrix} b_k \\ b_{-k}^+\end{pmatrix} \overset{\checkmark}{=} \begin{pmatrix} \beta_k \\ \beta_{-k}^+\end{pmatrix}.$

Exercise. $\epsilon_k = \hbar\omega_0\sqrt{1-\cos k}$, $\quad \dfrac{v_k}{u_k} = \dfrac{2-\cos k - 2\sqrt{1-\cos k}}{\cos k}$ (discuss this function!).

$$H = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\,\frac{\epsilon_k}{2}\big(\beta_k^+\beta_k + \beta_{-k}\beta_{-k}^+\big) = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\,\epsilon_k\,\beta_k^+\beta_k + E_0, \quad E_0 = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\,\frac{\epsilon_k}{2}.$$

Interpretation. $\beta_k|g.s.\rangle = 0$. The operator β_k^+ creates a stationary excitation (phonon or Bogoliubov quasi-particle) of momentum $\hbar k$ and energy ϵ_k:

$$e^{-itH/\hbar}\,\beta_k^+\,e^{itH/\hbar} = \beta_k^+\,e^{-it\epsilon_k/\hbar}.$$

Math background.

Recall: a_j^+, a_j $(j = 1, 2, \ldots, N)$ generate the Weyl algebra of $V \oplus V^*$, $V = \mathrm{span}_{\mathbb{C}}\{a_j^+\} \cong \mathbb{C}^N$, $V^* = \mathrm{span}_{\mathbb{C}}\{a_j\} \cong (\mathbb{C}^N)^*$.

Observation: the subspace spanned by the $N(2N+1)$ operators

$$a_j^+ a_{j'}^+ \,, \quad a_\ell a_{\ell'} \,, \quad a_j^+ a_\ell + a_\ell a_j^+ \qquad (j \leq j',\ \ell \leq \ell')$$

closes under the commutator. Thus it constitutes a Lie algebra.

Which Lie algebra?

Matrix representation. Consider (summation convention!)

$$\tfrac{1}{2} A^j{}_\ell (a_j^+ a^\ell + a^\ell a_j^+) + \tfrac{1}{2} B^{jj'} a_j^+ a_{j'}^+ - \tfrac{1}{2} C_{\ell\ell'} a^\ell a^{\ell'} \equiv \widehat{X} \,.$$

Consider also $\begin{pmatrix} A & B \\ C & -A^T \end{pmatrix} \equiv X$ for complex matrices A, B, C with $B^T = B$ and $C^T = C$.

Claim. The set of matrices X closes under commutation (thus it constitutes another Lie algebra) and $X \longmapsto \widehat{X}$ is an isomorphism of Lie algebras.

Main idea of proof.

$$\widehat{X} = \tfrac{1}{2} \begin{pmatrix} a_j^+ & -a^\ell \end{pmatrix} \begin{pmatrix} A^j{}_{\ell'} & B^{jj'} \\ C_{\ell\ell'} & -A^{j'}{}_\ell \end{pmatrix} \begin{pmatrix} a^{\ell'} \\ a_{j'}^+ \end{pmatrix} \equiv \tfrac{1}{2} \gamma_\nu X^\nu{}_{\nu'} \tilde{\gamma}^{\nu'} .$$

Use $[\tilde{\gamma}^\nu, \gamma_\mu] = \delta^\nu_\mu$ to show that $[\widehat{X}, \gamma_\mu] = \gamma_\nu X^\nu{}_\mu$. Then

$$[[\widehat{X}, \widehat{Y}], \gamma_\mu] \underset{\text{Jacobi}}{=} [\widehat{X}, [\widehat{Y}, \gamma_\mu]] - [\widehat{Y}, [\widehat{X}, \gamma_\mu]] \doteq \gamma_\nu [X, Y]^\nu{}_\mu$$

$$= [\widehat{[X,Y]}, \gamma_\mu] \quad \text{so} \quad [\widehat{X}, \widehat{Y}] = \widehat{[X,Y]} \ \bullet$$

Identification of Lie algebra. $(W_{\mathbb{C}} = W \otimes \mathbb{C})$

$$Sp(W_{\mathbb{C}}) = \{ g \in \mathrm{End}(W_{\mathbb{C}}) \mid \alpha(gw, gw') = \alpha(w, w') \text{ for all } w, w' \in W_{\mathbb{C}} \},$$

$$\mathrm{Lie}\, Sp(W_{\mathbb{C}}) = \{ X \in \mathrm{End}(W_{\mathbb{C}}) \mid \alpha(Xw, w') + \alpha(w, Xw') = 0 \},$$

$$\alpha(a^\ell, a_j^+) = \delta_j^\ell = \alpha(a_j^+, -a^\ell) \ \curvearrowright\ X = \begin{pmatrix} A & B \\ C & -A^T \end{pmatrix} \text{ as above } \bullet$$

More on the Exercise Sheet ...

III.10. Coherent-state path integral for bosons

Recall Chapter II: Feynman path integral for single-particle quantum mechanics.
Goal: develop the path integral for the many-particle quantum mechanics of bosons.

[For rigorous mathematics, see T. Balaban, J. Feldman, H. Knörrer, E. Trubowitz.]

III.10.a Coherent states

To describe the main idea, turn again to the 1D harmonic oscillator,

$$a = \frac{1}{\sqrt{2}}\left(\frac{q}{\ell} + \frac{i}{\hbar}\ell p\right), \quad a^+ = \frac{1}{\sqrt{2}}\left(\frac{q}{\ell} - \frac{i}{\hbar}\ell p\right), \quad \ell = \sqrt{\frac{\hbar}{m\omega}}, \quad [a, a^+] = 1,$$

and the ground state $|0\rangle$ satisfies $a|0\rangle = 0$ and $\langle 0| a^+ = 0$.

Coherent states are parametrized by a complex number z:

$$|z\rangle = \sum_{n=0}^{\infty} \frac{(z a^+)^n}{n!} |0\rangle \, e^{-\frac{1}{2}|z|^2} = \sum_{n=0}^{\infty} |n\rangle \frac{z^n}{\sqrt{n!}} e^{-\frac{1}{2}|z|^2},$$

$$\text{where } |n\rangle = \frac{(a^+)^n}{\sqrt{n!}} |0\rangle, \quad \langle m|n\rangle = \delta_{mn}.$$

Collection of formulas related to coherent states:

- $|z\rangle = T_z|0\rangle$, $T_z = e^{z a^+} e^{-\frac{1}{2}|z|^2} e^{-\bar{z} a} = e^{z a^+ - \bar{z} a}$,
  $T_z^\dagger = T_{-z} = T_z^{-1}$, i.e. T_z is a unitary operator.
- $\langle z|z'\rangle = \langle 0| T_z^\dagger T_{z'} |0\rangle = e^{-\frac{1}{2}|z|^2 + \bar{z} z' - \frac{1}{2}|z'|^2}$.
- $a T_z |0\rangle = T_z |0\rangle \cdot z$, $\langle 0| T_z^{-1} a^+ = \bar{z} \cdot \langle 0| T_z^{-1}$
  from $T_z^{-1} a T_z = a - [z a^+ - \bar{z} a, a] = a + z$, etc.

Nomenclature. The Heisenberg Lie algebra $\mathbb{C}a^+ \oplus \mathbb{C}a \oplus \mathbb{C}$ exponentiates to the Heisenberg group with multiplication law

$$T_u T_v = T_{u+v} \, e^{\frac{1}{2}(u\bar{v} - \bar{u}v)} = T_{u+v} \, e^{i\,\mathrm{Im}(u\bar{v})}.$$

That law follows from the Baker-Campbell-Hausdorff series,

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\dots}, \text{ which terminates here.}$$

Info. The Heisenberg group acts irreducibly on the Fock space $S(\mathbb{C}a^+)$.

III.10.b Resolution of unity by coherent states

Recall (from Chapter II) the resolution of the identity by $1 = \int dx\, |x\rangle\langle x|$.

Here we shall present an adaptation thereof to our bosonic case:

$$\boxed{\int_{\mathbb{C}} \frac{d^2z}{\pi}\, T_z |0\rangle\langle 0| T_z^{-1} = \mathcal{I}d_{\mathcal{F}}}\;, \qquad \mathcal{F} = S(\mathbb{C}a^+).$$

Normalization check: $\displaystyle\int_{\mathbb{C}} \frac{d^2z}{\pi} \langle 0|T_z|0\rangle\langle 0|T_z^{-1}|0\rangle = \int_{\mathbb{C}} \frac{d^2z}{\pi}\, e^{-|z|^2} \underset{\checkmark}{=} 1.$

$d^2z = d\,\mathrm{Re}(z)\, d\,\mathcal{I}m(z)$

<u>Proof</u> ("low tech").

$$\int_{\mathbb{C}} \frac{d^2z}{\pi} \langle m|T_z|0\rangle\langle 0|T_z^{-1}|n\rangle = \int_{\mathbb{C}} \frac{d^2z}{\pi}\, e^{-|z|^2} \frac{z^m}{\sqrt{m!}} \frac{\bar{z}^n}{\sqrt{n!}}$$

$$= \delta_{mn} \int_{\mathbb{C}} \frac{d^2z}{\pi} \frac{|z|^{2n}}{n!} e^{-|z|^2} = \delta_{mn} \int_0^\infty dr\, \frac{r^n}{n!} e^{-r} = \delta_{mn} \overset{\checkmark}{=} \langle m|\mathcal{I}d_{\mathcal{F}}|n\rangle.$$

<u>Proof</u> ("high tech").

$$T_w \int_{\mathbb{C}} \frac{d^2z}{\pi}\, T_z|0\rangle\langle 0|T_z^{-1} = \int_{\mathbb{C}} \frac{d^2z}{\pi}\, T_{w+z}|0\rangle\, e^{\frac{1}{2}(w\bar{z} - \bar{w}z)} \langle 0|T_z^{-1}$$

$$= \int_{\mathbb{C}} \frac{d^2z}{\pi}\, T_z|0\rangle\, e^{\frac{1}{2}(w\bar{z} - \bar{w}z)} \langle 0|T_{z-w}^{-1} = \int_{\mathbb{C}} \frac{d^2z}{\pi}\, T_z|0\rangle\langle 0|T_z^{-1}\, T_w.$$

Now,

$$\left\{ \begin{array}{l} \forall w:\; T_w\, Op = Op\, T_w\,, \\ \text{Heisenberg group acts} \\ \qquad\text{irreducibly on } \mathcal{F} \end{array} \right\} \xRightarrow[\text{Lemma}]{\text{Schur's}} Op = \text{const} \times \mathcal{I}d_{\mathcal{F}}\,,$$

and from the normalization check we know that const = 1. ■

III. 10.c Derivation of the path integral

Consider, e.g., the time-evolution trace, $\mathrm{Tr}_{\mathcal{F}}\, e^{-iT\hat{H}/\hbar}$.

First step: $\mathrm{Tr}\, e^{-iT\hat{H}/\hbar} = \lim_{N\to\infty} \mathrm{Tr}\left(e^{-i\frac{T}{N\hbar}\hat{H}}\right)^N$. Now use resolution of the identity (N times) and $\mathrm{Tr}\left(|0\rangle\langle 0|\, O_p\right) = \langle 0|\, O_p\,|0\rangle$ to express the time-evolution trace as

$$\mathrm{Tr}\, e^{-iT\hat{H}/\hbar} = \lim_{N\to\infty} \int_{\mathbb{C}} \frac{d^2 z_1}{\pi} \cdots \int_{\mathbb{C}} \frac{d^2 z_N}{\pi} \prod_{n=1}^{N} \langle 0|\, T^{\dagger}_{z_{n+1}}\, e^{-i\frac{T}{N\hbar}\hat{H}}\, T_{z_n} |0\rangle .$$

$z_{N+1} \equiv z_1$

Assume the Hamiltonian to be normal-ordered:

$\hat{H} = \hat{H}(a^+, a) = \text{const} + a^+ a + a^+ a^+ a a$ (schematic!) and use the relations $a\, T_{z_n}|0\rangle = T_{z_n}|0\rangle \cdot z_n$, $\langle 0|\, T^{-1}_{z_{n+1}}\, a^+ = \bar{z}_{n+1} \cdot \langle 0|\, T^{-1}_{z_{n+1}}$,

$$\langle 0|\, T^{-1}_{z_{n+1}} T_{z_n} |0\rangle = e^{-\frac{1}{2}|z_{n+1}|^2 - \frac{1}{2}|z_n|^2 + \bar{z}_{n+1} z_n}.$$ Then

$$\langle 0|\, T^{\dagger}_{z_{n+1}}\, e^{-i\frac{T}{N\hbar}\hat{H}(a^+, a)}\, T_{z_n}|0\rangle = e^{-i\frac{T}{N\hbar} H(\bar{z}_{n+1}, z_n) + \mathcal{O}((T/N)^2)} \times e^{-\frac{1}{2}|z_{n+1}|^2 - \frac{1}{2}|z_n|^2 + \bar{z}_{n+1} z_n}$$

and

$$\mathrm{Tr}\, e^{-iT\hat{H}/\hbar} = \lim_{N\to\infty} \prod_{n=1}^{N} \int_{\mathbb{C}} \frac{d^2 z_n}{\pi}\, e^{-\frac{1}{2}|z_{n+1}|^2 - \frac{1}{2}|z_n|^2 + \bar{z}_{n+1} z_n - i\frac{T}{N\hbar} H(\bar{z}_{n+1}, z_n)} .$$

$\Delta t = \frac{T}{N}$

Continuum approximation. $z_n \longrightarrow \varphi(t)$, $z_{n+1} \longrightarrow \varphi(t+\Delta t)$, $\bar{z}_n \longrightarrow \overline{\varphi(t)}$,

$$\frac{1}{2}|z_{n+1}|^2 + \frac{1}{2}|z_n|^2 - \bar{z}_{n+1} z_n \longrightarrow \frac{1}{2}|\varphi(t+\Delta t)|^2 + \frac{1}{2}|\varphi(t)|^2 - \overline{\varphi(t+\Delta t)}\,\varphi(t)$$

$$= \frac{1}{2}\overline{\varphi(t+\Delta t)}\left(\varphi(t+\Delta t) - \varphi(t)\right) - \frac{1}{2}\left(\overline{\varphi(t+\Delta t)} - \overline{\varphi(t)}\right)\varphi(t)$$

$$= \frac{1}{2}\Delta t\, \overline{\varphi(t)}\, \frac{\partial}{\partial t}\varphi(t) - \frac{1}{2}\Delta t\, \varphi(t)\, \frac{\partial}{\partial t}\overline{\varphi(t)} + \mathcal{O}((\Delta t)^2).$$

$\varphi(t) = \varphi(t+T)$

Hence $$\sum_{n=1}^{N}\left(\frac{1}{2}|z_{n+1}|^2 + \frac{1}{2}|z_n|^2 - \bar{z}_{n+1} z_n\right) \longrightarrow \int_0^T dt\, \overline{\varphi(t)}\, \frac{\partial}{\partial t}\varphi(t).$$

Similarly, $$\frac{T}{N}\sum_{n=1}^{N} H(\bar{z}_{n+1}, z_n) \longrightarrow \int_0^T dt\, H(\overline{\varphi(t)}, \varphi(t)).$$

Also, let $\prod_{n=1}^{N} \int_{\mathbb{C}} \frac{d^2 z_n}{\pi} \longrightarrow \mathcal{D}z$.

Final expression (continuum approximation to path integral for time-evolution trace)

$$\mathrm{Tr}\, e^{-iT\hat{H}/\hbar} = \int \mathcal{D}z\, e^{iS/\hbar},$$

$$S = \oint_0^T dt \left(i\hbar\, \overline{\varphi(t)}\, \frac{\partial}{\partial t}\varphi(t) - H(\overline{\varphi(t)}, \varphi(t)) \right).$$

Relation to Feynman path integral.

Consider, once again, the one-dimensional harmonic oscillator.

From $a = \frac{1}{\sqrt{2}}\left(\frac{\hat{q}}{\ell} + \frac{i}{\hbar}\ell\hat{p}\right)$, $a^+ = \frac{1}{\sqrt{2}}\left(\frac{\hat{q}}{\ell} - \frac{i}{\hbar}\ell\hat{p}\right)$, we infer that

$$\varphi(t) = \frac{1}{\sqrt{2}}\left(\frac{1}{\ell}q(t) + \frac{i}{\hbar}\ell\, p(t)\right), \quad \overline{\varphi(t)} = \frac{1}{\sqrt{2}}\left(\frac{1}{\ell}q(t) - \frac{i}{\hbar}\ell\, p(t)\right).$$

Thus $H(\overline{\varphi(t)}, \varphi(t)) = \hbar\omega\, |\varphi(t)|^2 = \frac{p(t)^2}{2m} + \frac{m}{2}\omega^2 q(t)^2$ and

$$i\hbar \oint_0^T dt\, \overline{\varphi(t)}\, \frac{\partial}{\partial t}\varphi(t) = \oint_0^T dt\, p(t)\frac{\partial}{\partial t}q(t). \text{ So,}$$

$$\mathrm{Tr}\, e^{-iT\hat{H}/\hbar} = \int \mathcal{D}q \int \mathcal{D}p\; e^{\frac{i}{\hbar}\oint_0^T dt \left(p(t)\frac{\partial}{\partial t}q(t) - \frac{p(t)^2}{2m} - \frac{m}{2}\omega^2 q(t)^2 \right)}.$$

Remark. The coherent-state path integral is secretly a phase-space path integral.

Reduction to Feynman PI:

$$\mathrm{Tr}\, e^{-iT\hat{H}/\hbar} = \int \mathcal{D}q\; e^{\frac{i}{\hbar}\oint_0^T dt \left(\frac{m}{2}\dot{q}(t)^2 - \frac{m}{2}\omega^2 q(t)^2 \right)} \times \int \mathcal{D}p\; e^{-\frac{i}{2m\hbar}\oint_0^T dt\, (p(t) - m\dot{q}(t))^2}.$$

Taking the integral over paths $t \mapsto p(t)$ in momentum space to be the inner integral, we can shift variables $p(t) \longrightarrow p(t) - m\dot{q}(t)$ and then perform the momentum-space path integral, which is Gaussian and gives simply a constant (independent of the position path $t \mapsto q(t)$). Thus we are left with Feynman's position-space path integral:

$$\mathrm{Tr}\, e^{-iT\hat{H}/\hbar} = \int \mathcal{D}q\; e^{\frac{i}{\hbar}\oint_0^T dt \left(\frac{m}{2}\dot{q}(t)^2 - \frac{m}{2}\omega^2 q(t)^2 \right)}.$$

Remark. This reduction goes through as long as the dependence of the Hamiltonian on the momentum is quadratic.

III. 11 Second quantization of two-body operators.

Recall that a one-body operator $L \equiv L^{(1)}$ is defined by $L : V \to V$ (single-particle Hilbert space V).

Now, a two-body operator $L \equiv L^{(2)}$ is defined by how its acts on two-particle states, $L : V \otimes V \longrightarrow V \otimes V$.

For some basis $\{e_i\}$ of V, let $\varphi_i(x)$ be the corresponding wave functions in the Schrödinger representation. Then the two-body matrix elements of L are calculated as

$$\langle ij | L | k\ell \rangle = \int d^3x \int d^3x' \; \overline{\varphi_i(x)}\; \overline{\varphi_j(x')} \left(L(\varphi_k \otimes \varphi_\ell) \right)(x, x').$$

Example (Coulomb interaction).

$$\left(U_C(\varphi_k \otimes \varphi_\ell) \right)(x, x') = \frac{e^2}{4\pi\varepsilon_0} \frac{\varphi_k(x)\,\varphi_\ell(x')}{|x - x'|}$$

$$\rightsquigarrow \langle ij | U_C | k\ell \rangle = \frac{e^2}{4\pi\varepsilon_0} \int d^3x \int d^3x' \; \frac{\overline{\varphi_i(x)\,\varphi_j(x')}\,\varphi_k(x)\,\varphi_\ell(x')}{|x - x'|}. \blacksquare$$

Write $L \in \mathrm{End}(V \otimes V) \cong (V \otimes V) \otimes (V^* \otimes V^*)$ in basis-independent form: $L = \frac{1}{2} \sum_{ijk\ell} (e_i \otimes e_j) \langle ij | L | k\ell \rangle (f^k \otimes f^\ell)$.

Remark. The factor $\frac{1}{2}$ is to avoid double-counting of pair interactions.

Second quantization now works as before:

We interpret L as a polynomial element in the Weyl algebra $\mathcal{W}(V \oplus V^*)$, and then pass to the representation of $\mathcal{W}(V \oplus V^*)$ on $S(V)$ by $e_i \mapsto \mu(e_i) = a_i^+$ and $f^k \mapsto \delta(f^k) = a^k$. Thus

$$L \longmapsto \hat{L} = \frac{1}{2} \sum_{ijk\ell} a_i^+ a_j^+ \langle ij | L | k\ell \rangle a^k a^\ell$$

$$= \frac{1}{4} \sum_{ijk\ell} a_i^+ a_j^+ \left(\langle ij | L | k\ell \rangle + \langle ij | L | \ell k \rangle \right) a^k a^\ell .$$

exchange matrix element

III.12 Quantization of the Electromagnetic Field

Common approach: electric scalar potential $\phi = 0$. Then $E_j = -\dot{A}_j$ ↝ treat the magnetic vector potential $\vec{A}$ as generalized positions and the electric field $\vec{E}$ as generalized momenta. Choose some gauge (e.g. Coulomb or "radiation" gauge, div $\vec{A} = 0$) to eliminate the unphysical degrees of freedom in $\vec{A}$.

Note: Coulomb gauge breaks relativistic covariance. Other gauges (e.g. Lorenz gauge) lead to issues with "states of negative norm".

Here we carry out the canonical quantization of the E.M. field in vacuum.

1. Phase space W (linear) = space of solutions of vacuum Maxwell equations:

$$\dot{B} = -\operatorname{rot} E = -\operatorname{rot} D/\varepsilon_0\,, \qquad \operatorname{div} D = 0 = \operatorname{div} B.$$
$$\dot{D} = +\operatorname{rot} H = +\operatorname{rot} B/\mu_0\,,$$

2. Symplectic structure / form α

$$\alpha(D,B;D',B') = \int d^3x \left(D' \cdot \operatorname{rot}^{-1} B - D \cdot \operatorname{rot}^{-1} B'\right) \quad \text{where}$$

$\operatorname{rot}^{-1} B = A$ is any vector potential such that $\operatorname{rot} A = B$.

α well defined (in particular, gauge-invariant)? Yes! Let $\operatorname{rot} A = \operatorname{rot} A' = B$.

Then $\int d^3x\, D \cdot (A - A') = \int d^3x\, D \cdot \operatorname{grad} f = -\int d^3x\, f \operatorname{div} D = 0$.

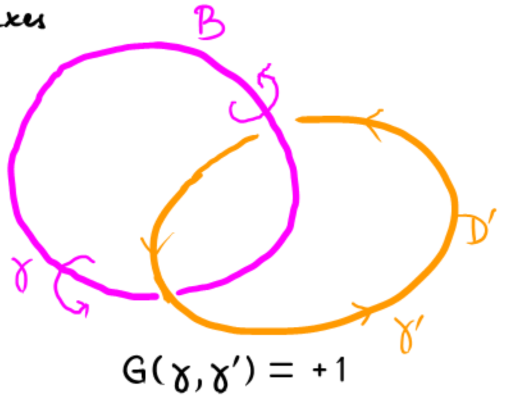
D assumed to vanish on boundary of domain

Info. By using the language of differential forms, one can write α in a way where relativistic covariance is manifest.

Remark. In Coulomb gauge ($\operatorname{div} A = 0$) one has

$$\int d^3x\, D' \cdot \operatorname{rot}^{-1} B = \int d^3x \int d^3y\, \frac{D'(x) \cdot \operatorname{rot} B(y)}{4\pi |x-y|}.$$

For special configurations where D' and B are confined to the interior of narrow tubes γ' and γ, this becomes $\int d^3x\, D' \cdot \operatorname{rot}^{-1} B = \Phi_{D'} \Phi_B\, G(\gamma,\gamma')$ where $\Phi_{D'} \Phi_B$ is the product of electric and magnetic fluxes (carried by the narrow tubes) and $G(\gamma,\gamma')$ is the Gauss linking number of the curves γ and γ'.



$G(\gamma,\gamma') = +1$

Exercise. Combined with the Hamiltonian function $H = \int d^3x \left(\frac{|D|^2}{2\varepsilon_0} + \frac{|B|^2}{2\mu_0}\right)$, the symplectic form α gives the proper equations of motion (Maxwell in vacuum).

3. Complex structure $\mathcal{J}$.

As before this will be phase flow by a quarter period. For good mathematical control, work on a bounded domain ("cavity") $\mathcal{U}$ with Dirichlet boundary conditions for the field components normal to the surface $\partial\mathcal{U}$. For generic $\mathcal{U}$, the spectrum of $-\Delta$ will be discrete and without multiplicity.

Given a solution D^λ of the Helmholtz equation $\left(\frac{\omega_\lambda^2}{c^2}+\Delta\right)D^\lambda = 0$ with characteristic frequency ω_λ, $\operatorname{div} D^\lambda = 0$, and $D_\perp^\lambda\Big|_{\partial\mathcal{U}} = 0$, put $B^\lambda = -\frac{\operatorname{rot} D^\lambda}{\omega_\lambda \varepsilon_0}$.

Then $D^\lambda = -\frac{\operatorname{rot} B^\lambda}{\omega_\lambda \mu_0}$, and

$$\phi_\lambda^{(1)} = \left(D^\lambda \cos(\omega_\lambda t),\, B^\lambda \sin(\omega_\lambda t)\right)$$

is a solution of Maxwell's equations, and so is

$$\phi_\lambda^{(2)} = \left(-D^\lambda \sin(\omega_\lambda t),\, B^\lambda \cos(\omega_\lambda t)\right).$$

The normal modes $\phi_\lambda^{(1)}$ and $\phi_\lambda^{(2)}$ span the two-dimensional space W_λ.
The complex structure $\mathcal{J}$ restricted to W_λ is given by

$$\begin{aligned}\mathcal{J}\,\phi_\lambda^{(1)} &= \left(D^\lambda \cos(\omega_\lambda t+\pi/2),\, B^\lambda \sin(\omega_\lambda t+\pi/2)\right)\\ &= \left(-D^\lambda \sin(\omega_\lambda t),\, +B^\lambda \cos(\omega_\lambda t)\right), \quad \text{and} \quad \mathcal{J}\,\phi_\lambda^{(2)} = -\phi_\lambda^{(1)}.\end{aligned}$$

Altogether, $W = \oplus_\lambda W_\lambda$ and $\mathcal{J} = \oplus_\lambda \mathcal{J}\big|_{W_\lambda}$.

Exercise. ⓘ α is time-independent.
(ii) $\mathcal{J}$ preserves α.

Check. $\mathcal{J}$ in conjunction with α determines a Euclidean structure on each of the normal-mode spaces W_λ:

$$g\left((D^\lambda, B^\lambda),(D^\lambda, B^\lambda)\right) = \alpha\left((D^\lambda, B^\lambda),\, \mathcal{J}(D^\lambda, B^\lambda)\right) = \frac{2}{\omega_\lambda} H(D^\lambda, B^\lambda) \geq 0. \checkmark$$

4. Polarization.

Decompose $W_\lambda \otimes \mathbb{C} = V_\lambda \oplus \tilde{V}_\lambda$, by the eigenspaces of J:

$$V_\lambda = E_{-i}(J) = \mathbb{C}\cdot\left(\phi^{(1)} + iJ\phi^{(1)}\right) = \mathbb{C}\cdot\left(\phi^{(1)} + i\phi^{(2)}\right),$$

$$\phi^{(1)} + i\phi^{(2)} = \Big(D^\lambda\left(\cos(\omega_\lambda t) - i\sin(\omega_\lambda t)\right),$$
$$B^\lambda\left(\sin(\omega_\lambda t) + i\cos(\omega_\lambda t)\right)\Big) = e^{-i\omega_\lambda t}\left(D^\lambda, iB^\lambda\right).$$

$$\tilde{V}_\lambda = E_{+i}(J) = \mathbb{C}\cdot\left(\phi^{(1)} - i\phi^{(2)}\right) = \mathbb{C}\cdot e^{+i\omega_\lambda t}\left(D^\lambda, -iB^\lambda\right).$$

5. Field quantization by mode expansion.

Decompose the general solution as

$$D(x,t) = \sum_\lambda D^\lambda(x)\left(c^\lambda e^{-i\omega_\lambda t} + \bar{c}_\lambda e^{+i\omega_\lambda t}\right),$$
$$B(x,t) = \sum_\lambda B^\lambda(x)\left(ic^\lambda e^{-i\omega_\lambda t} - i\bar{c}_\lambda e^{+i\omega_\lambda t}\right),$$

with complex coefficients c^λ and their complex conjugates $\bar{c}_\lambda$.

Single-photon Hilbert space $V = \bigoplus_\lambda V_\lambda$.

Reinterpret the coefficients as linear functions

$c^\lambda : V \longrightarrow \mathbb{C}$, $\bar{c}_\lambda : \tilde{V} \longrightarrow \mathbb{C}$ (i.e. $c^\lambda \in V^*$, $\bar{c}_\lambda \in \tilde{V}^* = \mathcal{I}(V)$).

[Recall the isomorphism $\mathcal{I} : V \longrightarrow \tilde{V}^*$, $v \longmapsto \frac{i}{\hbar}\alpha(v,\cdot)$.]

Multi-phonon Hilbert space (a.k.a. Fock space) $S(V)$.

Quantize by $c^\lambda \longmapsto \left\{\delta(c^\lambda) : S^n(V) \longrightarrow S^{n-1}(V)\right\}$

photon annihilation operator,

$\bar{c}_\lambda \longmapsto \left\{\mu\left(\mathcal{I}^{-1}(\bar{c}_\lambda)\right) : S^n(V) \longrightarrow S^{n+1}(V)\right\}$

photon creation operator.

5. Exercise. "Calibrate the Fock operators."

$$\frac{i}{\hbar}\alpha(\text{soln}, \text{soln}') = \sum_{\lambda} \frac{H(D^\lambda, B^\lambda)}{\hbar\omega_\lambda/2}\left(c^\lambda \bar{c}'_\lambda - \bar{c}_\lambda c'^\lambda\right),$$

$$H(D^\lambda, B^\lambda) = \int d^3x \left(\frac{|D^\lambda(x)|^2}{2\varepsilon_0} + \frac{|B^\lambda(x)|^2}{2\mu_0} \right).$$

$$\Longrightarrow \text{If } \left\{ \begin{aligned} a^\lambda &= \sqrt{\frac{H(D^\lambda, B^\lambda)}{\hbar\omega_\lambda/2}}\, \delta(c^\lambda) \\ a^+_\nu &= \sqrt{\frac{H(D^\nu, B^\nu)}{\hbar\omega_\nu/2}}\, \mu\left(\mathcal{I}^{-1}(\bar{c}_\nu)\right) \end{aligned} \right\}, \text{ then } [a^\lambda, a^+_\nu] = \delta^\lambda_\nu .$$

6. Quantized fields.

$$\hat{D}(x,t) = \sum_{\lambda} D^\lambda(x) \sqrt{\frac{\hbar\omega_\lambda/2}{H(D^\lambda, B^\lambda)}} \left(a^\lambda e^{-i\omega_\lambda t} + a^+_\lambda e^{i\omega_\lambda t} \right),$$

$$\hat{B}(x,t) = \sum_{\lambda} B^\lambda(x) \sqrt{\frac{\hbar\omega_\lambda/2}{H(D^\lambda, B^\lambda)}} \left(i a^\lambda e^{-i\omega_\lambda t} - i a^+_\lambda e^{i\omega_\lambda t} \right).$$

Quantum Hamiltonian:

$$\hat{H} = \int_{\mathcal{U}} d^3x \left(\frac{|\hat{D}(x,t)|^2}{2\varepsilon_0} + \frac{|\hat{B}(x,t)|^2}{2\mu_0} \right) = \sum_{\lambda} \frac{\hbar\omega_\lambda}{2} \left(a^+_\lambda a^\lambda + a^\lambda a^+_\lambda \right)$$

(needs normal ordering,
Casimir effect, ...) ∎

Chapter IV : Fermions

IV.1 Grassmann algebra & Clifford algebra

Wave functions for identical fermions are totally skew (or anti-symmetric). Here assume the existence of a particle picture with single-particle Hilbert space V, dual V^*. Hermitian scalar product $\langle \cdot , \cdot \rangle_V$.

Frechet-Riesz isomorphism $\gamma_V : V \longrightarrow V^*$, $v \longmapsto \langle v, \cdot \rangle_V$.

Physics notation (Dirac).

Orthonormal basis $|i\rangle \longrightarrow c_i^+$,

dual basis $\langle i | \longrightarrow c^i$.

Canonical anticommutation relations (CAR) :

$$c_i^+ c_j^+ + c_j^+ c_i^+ = 0 = c^i c^j + c^j c^i , \qquad c^i c_j^+ + c_j^+ c^i = \delta^i_j .$$

Fermionic Fock space $\mathcal{F} = \bigoplus_{n \geqslant 0} \mathcal{F}^n$ (n = particle number),

$\mathcal{F}^0 = |0\rangle \cdot \mathbb{C}$, $\mathcal{F}^1 = \mathrm{span}_{\mathbb{C}} \{ c_i^+ |0\rangle \}$, ..., $\mathcal{F}^n = \mathrm{span}_{\mathbb{C}} \{ c_{i_1}^+ c_{i_2}^+ \cdots c_{i_n}^+ |0\rangle \}$, ...

creation operators $c_i^+ : \mathcal{F}^n \longrightarrow \mathcal{F}^{n+1}$,

annihilation operators $c^i : \mathcal{F}^n \longrightarrow \mathcal{F}^{n-1}$, $c^i |0\rangle = 0$.

Second quantization of one-body operators :

$$L = \sum_{ij} |i\rangle\langle i | L | j \rangle\langle j| \longrightarrow \hat{L} = \sum_{ij} \langle i | L | j \rangle \, c_i^+ c^j .$$

See below for the Hermitian scalar product on $\mathcal{F}$.

Invariant formulation (→ universal algebraic structure).

Definition. For a complex vector space V, the **exterior (or Grassmann) algebra** $\Lambda(V)$ is the associative algebra generated by $V \oplus \mathbb{C}$ with relations $v v' + v' v = 0$ (for all $v, v' \in V$).

Remark. $v v' \equiv v \wedge v' = - v \wedge v'$ (exterior product),

$\leadsto$ $v^2 = v \wedge v = - v \wedge v = 0$ (Pauli principle).

Fermionic Fock space $\mathcal{F} = \Lambda(V)$. Transcription:

$$\Lambda^0(V) = \mathbb{C} \ni 1 \longleftrightarrow |0\rangle \in \mathcal{F}^0, \quad \Lambda^1(V) = V \ni v = e_i v^i \longleftrightarrow c_i^+|0\rangle v^i \in \mathcal{F}^1.$$

Exercise. $\dim \Lambda^n(\mathbb{C}^N) = \binom{N}{n}$.

Hermitian structure of $\Lambda(V)$ inherited from V:

$$\langle v_1 v_2 \cdots v_n , v_1' v_2' \cdots v_n' \rangle_{\Lambda^n(V)} = \sum_{\pi \in S_n} \text{sign}(\pi) \langle v_1 , v'_{\pi(1)} \rangle_V \langle v_2 , v'_{\pi(2)} \rangle_V \cdots \langle v_n , v'_{\pi(n)} \rangle_V$$

$$= \text{Det} \begin{pmatrix} \langle v_1 , v_1' \rangle_V & \cdots & \langle v_1 , v_n' \rangle_V \\ \vdots & \ddots & \vdots \\ \langle v_n , v_1' \rangle_V & \cdots & \langle v_n , v_n' \rangle_V \end{pmatrix}.$$

Transcription to physics notation. Orthonormal basis $\{e_i\}$ of V.

$$1 \equiv |0\rangle, \quad e_i \equiv c_i^+|0\rangle, \quad e_i e_j \equiv c_i^+ c_j^+|0\rangle, \quad \text{etc.}$$

Let $\Psi = c_{i_1}^+ c_{i_2}^+ \cdots c_{i_n}^+|0\rangle$ and $\Psi' = c_{i_1'}^+ c_{i_2'}^+ \cdots c_{i_n'}^+|0\rangle$.

Then $\langle \Psi | \Psi' \rangle = \langle 0 | c^{i_n} \cdots c^{i_2} c^{i_1} \, c_{i_1'}^+ c_{i_2'}^+ \cdots c_{i_n'}^+ |0\rangle$

$$= \sum_{\pi \in S_n} \text{sign}(\pi) \, \delta^{i_1}{}_{i'_{\pi(1)}} \, \delta^{i_2}{}_{i'_{\pi(2)}} \cdots \delta^{i_n}{}_{i'_{\pi(n)}} . \blacksquare$$

Question: What takes the role of the Weyl algebra (→ bosons) in the present case of fermions?

Definition. Let V be a complex vector space. The **Clifford algebra** $Cl(V \oplus V^*)$ is the associative algebra generated by $V \oplus V^* \oplus \mathbb{C}$ with relations

$$v v' + v' v = 0, \quad \varphi \varphi' + \varphi' \varphi = 0, \quad \varphi v + v \varphi = \varphi(v) \cdot 1$$

(for all $v, v' \in V$ and $\varphi, \varphi' \in V^*$).

Operations on $\Lambda(V)$.

i. **Exterior multiplication** $\varepsilon(v) : \Lambda^n(V) \longrightarrow \Lambda^{n+1}(V) \qquad (v \in V),$

$$\Psi \longmapsto v \wedge \Psi = (-1)^n \, \Psi \wedge v \, .$$

ii. **Alternating derivation** $\iota(\varphi) : \Lambda^n(V) \longrightarrow \Lambda^{n-1}(V) \qquad (\varphi \in V^*)$

defined by $\iota(\varphi) \cdot 1 = 0$, $\iota(\varphi) \cdot v = \varphi(v) \in \mathbb{C}$,

$\iota(\varphi) \cdot (v v') = \varphi(v) \, v' - \varphi(v') \, v$ & continue by the Leibniz product rule with alternating sign.

Transcription. $\varepsilon(v) \longleftrightarrow c_i^{+} v^i$ creation op.

$\iota(\varphi) \longleftrightarrow \varphi_i \, c^i$ annihilation op.

Exercise. $\varepsilon(v)\varepsilon(v') + \varepsilon(v')\varepsilon(v) = 0 = \iota(\varphi)\iota(\varphi') + \iota(\varphi')\iota(\varphi)$,

$\iota(\varphi)\varepsilon(v) + \varepsilon(v)\iota(\varphi) = 1_{\Lambda(V)} \cdot \varphi(v)$.

Corollary. The Clifford algebra $Cl(V \oplus V^*)$ acts on the exterior algebra $\Lambda(V)$ by $V \oplus V^* \ni v + \varphi \longmapsto \varepsilon(v) + \iota(\varphi)$.

Fact. Second quantization of one-body operators,

$$L \longmapsto \varepsilon(L e_i)\, \iota(f^i) \equiv \hat{L} \, ,$$

preserves commutators : $[\hat{L}, \hat{M}] = \widehat{[L, M]}$.

Hermitian conjugation. (Frechet-Riesz isomorphism γ)

$$\begin{tikzcd} \Lambda^n(V) \arrow[r, shift left, "\varepsilon(v)"] & \Lambda^{n+1}(V) \arrow[l, shift left, "\varepsilon(v)^{+} = \iota(\gamma v)"] \end{tikzcd} , \qquad \begin{tikzcd} \Lambda^n(V) \arrow[r, shift left, "\iota(\varphi)"] & \Lambda^{n-1}(V) \arrow[l, shift left, "\iota(\varphi)^{+} = \varepsilon(\gamma^{-1}\varphi)"] \end{tikzcd} , \; .$$

Outlook. The invariant formulation will be instrumental in the quantization of the Dirac field .

IV. 2 Dirac equation (quick summary).

Dirac (1928) combines quantum mechanics with special relativity:

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \quad \text{where} \quad H = \beta mc^2 + c\sum_{j=1}^{3} \alpha_j (p_j - eA_j) + e\phi$$

acts on spinor fields $\psi \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$. Clifford algebra relations:

$$\beta^2 = 1, \quad \beta\alpha_j + \alpha_j\beta = 0, \quad \alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij} \quad (i,j = 1,2,3).$$

Standard representation: $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}$.

Gauge potentials: $E_i = -\partial_i\phi - \partial_t A_i$, $B_{ij} = \partial_i A_j - \partial_j A_i$.

Continuity equation: $\frac{\partial}{\partial t}\rho + \operatorname{div}\vec{j} = 0$, where
$\rho = \psi^{\dagger}\psi$, $\vec{j} = c\,\psi^{\dagger}\vec{\alpha}\psi$.

Interpretation of ρ as probability density fctn
and $\vec{j}$ as probability current vector field? NO!

Problems. Standard second quantization

$$H \longrightarrow \sum_{n,n'} \langle n|H|n'\rangle\, c_n^{+} c_{n'} = \widehat{H} \quad \text{on } \Lambda(V)$$

with $V = L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ leads to unphysical behavior when the Dirac field is coupled to the electromagnetic field. The source of the problem is that the (free) Dirac Hamiltonian has positive spectrum $E \geqslant +mc^2$ but also negative spectrum $E \leqslant -mc^2$ and thus is <u>not</u> bounded from below. By consequence, $\widehat{H}$ does not have a ground state (!) and in the interacting system the energy stored in the Dirac matter may go to $-\infty$ while the energy of the electromagnetic field goes to $+\infty$.

Klein paradox (→ exercise). A low-energy electron incident on a potential step $e\,\Delta\phi > 2mc^2$ scatters (according to the time-independent Dirac equation) to a reflected and a transmitted wave, with reflection probability $|r|^2 > 1$.

Remark. In the final formulation of the Dirac theory the apparent problem is resolved by re-interpreting the continuity equation $\frac{\partial}{\partial t}\rho + \operatorname{div}\vec{j} = 0$ as the law of **charge conservation** (*not* conservation of probability). In particular, $\rho = \psi^\dagger \psi$ (after normal ordering with respect to the true vacuum) may become negative.

IV.3 Hole quantization

Recall standard (particle-type) quantization:

$$V \ni v \mapsto \varepsilon(v) : \Lambda^n(V) \longrightarrow \Lambda^{n+1}(V) \qquad \text{creation op.}$$

$$V^* \ni \varphi \mapsto \iota(\varphi) : \Lambda^n(V) \longrightarrow \Lambda^{n-1}(V) \qquad \text{annihilation op.}$$

$$\mathrm{End}(V) = V \otimes V^* \ni H = (He_i) \otimes f^i \mapsto \varepsilon(He_i) \otimes \iota(f^i) = {}^p\widehat{H}.$$

Alternative (**hole-type**) quantization:

Replace the Fock space $\Lambda(V)$ by the Fock space $\Lambda(V^*)$. Then

$$V \ni v \mapsto \iota(v) : \Lambda^n(V^*) \longrightarrow \Lambda^{n-1}(V^*) \qquad \text{annihilation op.}$$

$$V^* \ni \varphi \mapsto \varepsilon(\varphi) : \Lambda^n(V^*) \longrightarrow \Lambda^{n+1}(V^*) \qquad \text{creation op.}$$

$$\mathrm{End}(V) = V \otimes V^* \ni H = (He_i) \otimes f^i \mapsto \iota(He_i) \otimes \varepsilon(f^i) + \text{const}$$
$$= -\varepsilon(f^i) \otimes \iota(He_i) = \varepsilon(-H^t f^i) \otimes \iota(e_i) = {}^h\widehat{H}.$$

Remark. The two schemes are on the same footing from a purely algebraic viewpoint (both are Lie algebra homomorphisms),

BUT if $H > 0$ then $H \mapsto {}^p\widehat{H}$

WHILE if $H < 0$ then $H \mapsto {}^h\widehat{H}$

is the "good" scheme to use.

Comparison with Dirac sea picture. Recall $V \oplus V^* \ni v + \varphi$.

$$\Lambda(V) \curvearrowleft \varepsilon(v) + \iota(\varphi) \underset{\text{part.-Q.}}{\longleftarrow\!\!\shortmid} v + \varphi \underset{\text{hole-Q.}}{\longmapsto} \iota(v) + \varepsilon(\varphi) \curvearrowright \Lambda(V^*)$$

Cartoon. $\bullet$ occupied s.p. state $\quad \circ$ empty s.p. state

$$\begin{array}{cccccc} n = & 1 & 2 & 3 & 4 & 5 \\ & \bullet & \bullet & \bullet & \circ & \bullet \end{array}$$

Note: $c_1^+ c_2^+ c_3^+ c_5^+ |0\rangle \longleftrightarrow c_4 |\text{full}\rangle$ "Dirac sea"

$\langle 1| \equiv \varphi \in V^*$: $\underset{\text{annihilates particle}}{c_1 \equiv \iota(\varphi)} \longleftrightarrow \underset{\text{creates hole}}{\varepsilon(\varphi) \equiv c_1}$

$|4\rangle \equiv v \in V$: $\underset{\text{creates particle}}{c_4^+ \equiv \varepsilon(v)} \longleftrightarrow \underset{\text{annihilates hole}}{\iota(v) \equiv c_4^+}$

Warning: the correspondence becomes problematic for $\dim V = \infty$. Yet, hole quantization continues to exist and make immediate sense, whereas the Dirac sea picture becomes somewhat of a fairy tale.

[Filled Dirac sea with infinite charge & energy? Casimir effect ??]

H_0-stable quantization.

Let $H_0 = H(\phi = 0, \vec{A} = 0)$ be the free part of the Dirac Hamiltonian.

Make eigenspace decomposition: $V = E_{>0}(H_0) \oplus E_{<0}(H_0) \equiv V_+ \oplus V_-$.

Building on the Fock space $\Lambda(V_+ \oplus V_-^*)$, adopt the hybrid scheme

$$V_+ \oplus V_- \oplus V_+^* \oplus V_-^* \ni v_+ + v_- + \varphi_+ + \varphi_-$$
$$\mapsto \varepsilon(v_+) + \iota(v_-) + \iota(\varphi_+) + \varepsilon(\varphi_-).$$

Then $H_0 \gtrless 0 \mapsto \widehat{H}_0 > 0$ (stability $\rightsquigarrow$ ground state exists).

The charge conjugation "mystery" (as a teaser).

Fact 1. If $i\hbar \frac{\partial \psi}{\partial t} = H(\phi, \vec{A})\,\psi$ then

$$i\hbar \frac{\partial \psi^c}{\partial t} = H(-\phi, -\vec{A})\,\psi^c \quad \text{for } \psi^c = \beta \alpha_2 \overline{\psi} \equiv C\psi .$$

Remark. This is known as the charge conjugation symmetry of the Dirac equation (cf. B. Thaller: The Dirac equation, Springer 1992).

Note that the mapping $\psi \mapsto C\psi$ is complex antilinear.

Fact 2. Textbooks on QFT (cf. S. Weinberg: The Quantum Theory of Fields, vol. 1, Cambridge University Press 1995) state that charge conjugation is a unitary (hence complex linear) symmetry of, e.g., quantum electrodynamics.

Comment: CPT–Theorem.

IV.4 Canonical quantization of the Dirac field.

[Go beyond the Dirac sea picture.]

① Textbook treatment.

To construct the general solution of the Dirac equation, first pass to the relativistic ("covariant") formulation.

Recall $i\hbar \frac{\partial}{\partial t}\psi = \left(\beta m c^2 + \frac{\hbar c}{i}\sum_{j=1}^{3} \alpha_j \frac{\partial}{\partial x^j}\right)\psi .$

Introduce $\gamma^0 \equiv \beta$, $\gamma^j = \beta\alpha_j$ $(j=1, 2, 3)$, $x^0 = ct$. Multiply the Dirac equation by $\frac{\beta}{\hbar c}$. Then

$$\boxed{D\psi = 0, \quad D = -i\gamma^\mu \frac{\partial}{\partial x^\mu} + \frac{mc}{\hbar} .}$$

$mc/\hbar$ is called the Compton wave number of the Dirac particle with mass m.

- Plane-wave ansatz for the solution ψ :

$\psi = u(k)\, e^{ik\cdot x}$, $u(k) \in \mathbb{C}^4$, $k\cdot x = k_\mu x^\mu$, $k_0 \equiv -\omega/c$.

Then $D\psi = 0 \implies \left(\gamma^\mu k_\mu + \frac{mc}{\hbar}\right) u(k) = 0$ $\leadsto$ secular equation:

$$0 = \mathrm{Det}\left(\gamma^\mu k_\mu + \frac{mc}{\hbar}\right) = \mathrm{Det}\begin{pmatrix} \frac{mc}{\hbar} - \frac{\omega}{c} & \sum k_j \sigma_j \\ -\sum k_j \sigma_j & \frac{mc}{\hbar} + \frac{\omega}{c} \end{pmatrix}.$$

Now use $\mathrm{Det}\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \mathrm{Det}(A)\, \mathrm{Det}(D - CA^{-1}B)$
$= \mathrm{Det}(A - BD^{-1}C)\, \mathrm{Det}(D)$

and $\left(\sum_{j=1}^{3} k_j \sigma_j\right)^2 = \sum_{jl} k_j k_l \frac{1}{2}(\sigma_j \sigma_l + \sigma_l \sigma_j) = 1_2 \cdot \sum_j k_j^2 \equiv |k|^2\, 1$

to bring the secular equation into the form

$$0 = \left(-\left(\frac{\omega}{c}\right)^2 + \left(\frac{mc}{\hbar}\right)^2 + |k|^2\right)^2.$$

The positive-frequency solution $\omega(k) = +c\sqrt{\left(\frac{mc}{\hbar}\right)^2 + |k|^2}$ has multiplicity 2 (→ spin degeneracy):

$$\left(-\gamma^0 \frac{\omega(k)}{c} + \gamma^j k_j + \frac{mc}{\hbar}\right) u_s(k) = 0, \quad s = \pm\frac{1}{2}.$$

Positive-frequency spinors in the rest frame (of the Dirac particle), i.e. for $|k|^2 = 0$, or $\hbar\omega = mc^2$: $u_{+\frac{1}{2}}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, $u_{-\frac{1}{2}}(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$.

Away from the rest frame, spinors are normalized by the condition $u_s(k)^\dagger \gamma^0 u_{s'}(k) = \delta_{ss'}$, using the dagger operation $\mathbb{C}^4 \xrightarrow{\dagger} (\mathbb{C}^4)^*$.

[Motivation: this normalization condition is Lorentz-invariant; see later.]

- In order to obtain a complete system of linearly independent solutions (while insisting on $\omega(k) > 0$) we make a second plane-wave ansatz:

$\psi^- = v(k)\, e^{-ik\cdot x}$, $v(k) \in \mathbb{C}^4$, $-k_0 c = \omega > 0$.

Then $D\psi^- = 0 \implies \left(-\gamma^\mu k_\mu + \frac{mc}{\hbar}\right) v(k) = 0$.

Still with $\omega(k) = c\sqrt{\left(\frac{mc}{\hbar}\right)^2 + |k|^2} > 0$, we then have negative-energy spinors $v_s(k)$, which satisfy $\left(\gamma^0 \frac{\omega(k)}{c} + \gamma^j k_j + \frac{mc}{\hbar}\right) v_s(k) = 0$, $s = \pm\frac{1}{2}$.
In the rest frame they are expressed as $v_{+\frac{1}{2}}(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$, $v_{-\frac{1}{2}}(0) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$.
<u>Notice</u> $\frac{\hbar}{i}\frac{\partial}{\partial x^l} e^{-ik\cdot x} = -\,\hbar k_l\, e^{-ik\cdot x}$ and $S^3 v_s(k) = -\,\hbar s\, v_s(k)$.
The Lorentz-invariant normalization condition is $v_s(k)^\dagger \gamma^0 v_{s'}(k) = -\delta_{ss'}$.

Exercise. 1. $\sum_s u_s(k)\, u_s(k)^\dagger \gamma^0 - \sum_s v_s(k)\, v_s(k)^\dagger \gamma^0 = 1_{4\times 4}$ ("completeness"),

2. $u_s(k)^\dagger u_{s'}(k) = \delta_{ss'} \sqrt{\frac{\hbar\omega(k)}{mc^2}} = v_s(k)^\dagger v_{s'}(k)$ ("orthogonality").

- By superposition of the positive- and negative-energy solutions, we expand the general solution $\psi(x) \equiv \psi(\vec{x}, t)$ as

$$\psi(x) = \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{mc^2}{\hbar\omega(k)}} \sum_s \left(u_s(k)\, e^{+ik\cdot x} c_s^+(k) + v_s(k)\, e^{-ik\cdot x} c_s^-(k) \right)$$

with complex coefficients $c_s^+(k)$ and $c_s^-(k)$.

<u>Remark</u>. The integration measure $\propto d^3k \sqrt{\frac{mc^2}{\hbar\omega(k)}}$ can be motivated by Lorentz invariance and/or by Exercise 2. (above) in conjunction with formulas that will appear below. (More constructively, it emerges from the fermionic version of canonical quantization.)

- <u>Stop</u> to count: For fixed k, the expression for the solution ψ has 4 independent degrees of freedom over $\mathbb{C}$ (namely, $c_s^+(k)$ and $c_s^-(k)$). On physical grounds, we expect 8 complex freedoms due to 2 (e^-/e^+) × 2 (spin) × 2 (create/annihilate). In order to produce the 4 missing freedoms, one takes the Hermitian conjugate:

$$\psi^+(x) := \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{mc^2}{\hbar\omega(k)}} \sum_s \left(\overline{c_s^+(k)}\, e^{-ik\cdot x} u_s(k)^\dagger + \overline{c_s^-(k)}\, e^{+ik\cdot x} v_s(k)^\dagger \right)$$

and later views $\overline{c_s^+(k)}$ and $\overline{c_s^-(k)}$ (in the sense of complex polarization) as independent of $c_s^+(k)$ resp. $c_s^-(k)$.

[Remark. Mathematically speaking, the operation $\psi \longmapsto \psi^+$ is well-defined only if the spinor bundle $S \xrightarrow{\pi} M$ (= space), $\pi^{-1}(x) \cong \mathbb{C}^4$, carries a Hermitian structure. It is not clear a priori how the physics of the Dirac equation (as a classical wave equation) provides such a structure.]

- **Field Quantization.**

Let $V_{+(-)} = \mathrm{span}_{\mathbb{C}}$ of the positive (negative) energy solutions. Let Fock space $= \Lambda(V_+ \oplus V_-^*)$. Re-interpret the coefficients $c_s^\pm(k)$ as linear functions, $c_s^+(k) \in V_+^*$ and $c_s^-(k) \in V_-^*$. Then

$$\hat{\psi}(x) = \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{mc^2}{\hbar\omega(k)}} \sum_s \Big(u_s(k)\, e^{+ik\cdot x}\, \iota(c_s^+(k)) + v_s(k)\, e^{-ik\cdot x}\, \varepsilon(c_s^-(k)) \Big).$$

Remark. $\begin{cases} \iota(c_s^+(k)) \text{ annihilates an electron with momentum } \hbar\vec{k} \text{ and spin } \hbar s, \\ \varepsilon(c_s^-(k)) \text{ creates a positron with momentum } \hbar\vec{k} \text{ and spin } \hbar s. \end{cases}$

And

$$\hat{\psi}^+(x) = \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{mc^2}{\hbar\omega(k)}} \sum_s \Big(\varepsilon\big(\overline{c_s^+(k)}\big)\, e^{-ik\cdot x}\, u_s(k)^\dagger + \iota\big(\overline{c_s^-(k)}\big)\, e^{+ik\cdot x}\, v_s(k)^\dagger \Big).$$

Here the coefficients $\overline{c_s^\pm(k)}$ are re-interpreted as elements $\overline{c_s^+(k)} \in V_+$ and $\overline{c_s^-(k)} \in V_-$, but it is left open exactly how that should be done. Anyway,

$\varepsilon\big(\overline{c_s^+(k)}\big)$ creates an electron with momentum $\hbar\vec{k}$ and spin $\hbar s$,

$\iota\big(\overline{c_s^-(k)}\big)$ annihilates a positron with momentum $\hbar\vec{k}$ and spin $\hbar s$.

The (nonvanishing) canonical anticommutation relations are

$$\iota(c_s^+(k))\, \varepsilon\big(\overline{c_{s'}^{+\prime}(k')}\big) + \varepsilon\big(\overline{c_{s'}^{+\prime}(k')}\big)\, \iota(c_s^+(k)) = (2\pi)^3 \delta(k-k')\, \delta_{ss'},$$

$$\iota\big(\overline{c_s^-(k)}\big)\, \varepsilon(c_{s'}^{-\prime}(k')) + \varepsilon(c_{s'}^{-\prime}(k'))\, \iota\big(\overline{c_s^-(k)}\big) = (2\pi)^3 \delta(k-k')\, \delta_{ss'}.$$

Exercises.

- Equal-time anticommutation relations:

$$\hat{\psi}^{a'}(\vec{x}',t)\,\hat{\psi}^{+}_{a}(\vec{x},t)+\hat{\psi}^{+}_{a}(\vec{x},t)\,\hat{\psi}^{a'}(\vec{x}',t)=\delta^{a'}_{a}\,\delta(\vec{x}-\vec{x}').$$

- Total charge:

$$\hat{Q}=e\int d^3x\;:\hat{\psi}^{+}_{a}(\vec{x},t)\,\hat{\psi}^{a}(\vec{x},t):$$
$$=\int\frac{d^3k}{(2\pi)^3}\sum_s\Big(\varepsilon\big(\overline{c^{+}_{s}(k)}\big)\,\iota\big(c^{+}_{s}(k)\big)-\varepsilon\big(c^{-}_{s}(k)\big)\,\iota\big(\overline{c^{-}_{s}(k)}\big)\Big).$$

- Total energy:

$$\hat{H}=i\hbar\int d^3x\;:\hat{\psi}^{+}_{a}(\vec{x},t)\,\frac{\partial}{\partial t}\,\hat{\psi}^{a}(\vec{x},t):$$
$$=\int\frac{d^3k}{(2\pi)^3}\sum_s\hbar\omega(k)\Big(\varepsilon\big(\overline{c^{+}_{s}(k)}\big)\,\iota\big(c^{+}_{s}(k)\big)+\varepsilon\big(c^{-}_{s}(k)\big)\,\iota\big(\overline{c^{-}_{s}(k)}\big)\Big).$$

- Total momentum:

$$\hat{P}_j=-i\hbar\int d^3x\;:\hat{\psi}^{+}_{a}(\vec{x},t)\,\frac{\partial}{\partial x_j}\,\hat{\psi}^{a}(\vec{x},t):$$
$$=\int\frac{d^3k}{(2\pi)^3}\sum_s\hbar k_j\Big(\varepsilon\big(\overline{c^{+}_{s}(k)}\big)\,\iota\big(c^{+}_{s}(k)\big)+\varepsilon\big(c^{-}_{s}(k)\big)\,\iota\big(\overline{c^{-}_{s}(k)}\big)\Big).$$

② Beyond textbook ...

- View the Dirac equation as a classical wave-type equation.
- Quantize the Dirac field by a procedure of canonical quantization.

The input data required for fermions are

1. A (complex) phase space $W_{\mathbb{C}}$ with real structure $W_{\mathbb{R}}\subset W_{\mathbb{C}}$;
2. A symmetric complex bilinear form $B: W_{\mathbb{C}}\otimes W_{\mathbb{C}}\longrightarrow\mathbb{C}$;
3. A complex structure $J\in\mathrm{End}(W_{\mathbb{R}})$ compatible with B.

See QFT1-Lecture_30 for more information.

IV.5 Berezin integral

① Naive picture (one degree of freedom).

$V^* = \mathbb{C}\cdot\xi$ (Grassmann variable ξ, $\xi^2 = 0$).

superfunction $f = f_0 + f_1\xi \in \Lambda(V^*)$.

$\int_F f := f_1$, i.e. $\int d\xi\cdot 1 = 0$ and $\int d\xi\cdot\xi = 1$.

Note $\int d\xi \equiv \frac{\partial}{\partial\xi}$ (bad notation $d\xi$).

② Informed picture.

Ordinary integration: $x^k \underset{\int dx}{\overset{d/dx}{\rightleftarrows}} k\,x^{k-1}$,

more generally $S^k(V^*) \xrightarrow{\delta(v)} S^{k-1}(V^*)$ $(v \in V)$.

Note $\int_{\text{closed}} \delta(v) f = 0$ (for translation-invariant integration measure).

Fermionic integration (Berezin) is a linear function $\int_F : \Lambda(V^*) \to \mathbb{C}$.

Recall contraction $\Lambda^k(V^*) \xrightarrow{\iota(v)} \Lambda^{k-1}(V^*)$ $(v \in V)$.

Demand $\int \iota(v)\psi = 0$ (∼ "translation invariance").

Solution: if $\dim V = n$, pick $\Omega \in \Lambda^{\text{top}}(V)$, say

$\Omega = c\, e_n \wedge e_{n-1} \wedge \cdots \wedge e_2 \wedge e_1$ for some basis $\{e_i\}$ of V.

Then define $\int_F \psi = \Omega[\psi] \equiv c\,\iota(e_n)\,\iota(e_{n-1})\cdots\iota(e_1)\,\psi$.

Standard notation. Basis $\{e_\mu\}$ of V, dual basis $\{f^\mu\}$ of V^*.

$\varepsilon(f^\mu) \equiv \xi^\mu$ (generators of $\Lambda(V^*)$), $\iota(e_\mu) = \frac{\partial}{\partial\xi^\mu}$.

CAR: $\frac{\partial}{\partial\xi^\nu}\xi^\mu + \xi^\mu\frac{\partial}{\partial\xi^\nu} = \delta^\mu_\nu$, $\xi^\nu\xi^\mu + \xi^\mu\xi^\nu = 0 = \frac{\partial}{\partial\xi^\nu}\frac{\partial}{\partial\xi^\mu} + \frac{\partial}{\partial\xi^\mu}\frac{\partial}{\partial\xi^\nu}$.

If $\dim V = N$, the general element of $\Lambda(V^*)$ is a polynomial of order N:

$$f = f^{(0)} + \sum_{\mu=1}^{N} f^{(1)}_\mu \xi^\mu + \sum_{\mu<\nu} f^{(2)}_{\mu\nu}\xi^\mu\xi^\nu + \sum_{\mu<\nu<\lambda} f^{(3)}_{\mu\nu\lambda}\xi^\mu\xi^\nu\xi^\lambda + \cdots + f^{(N)}_{12\cdots N}\xi^1\xi^2\cdots\xi^N.$$

Definition (Grassmann integral): $\int_F f := f^{(N)}_{12\cdots N} = \frac{\partial^N}{\partial\xi^N\cdots\partial\xi^2\partial\xi^1} f$.

Remark. Grassmann integration is nothing but differentiation!

IV.6 Determinant and Pfaffian as Berezin integrals

Example (Gauss integral).

$W = V \oplus V^*$, $\dim V = N$. $\Lambda(W^*) \simeq \Lambda(V^*) \otimes \Lambda(V)$.

$\zeta^1, \dots, \zeta^N$ generators of $\Lambda(V^*)$; $\bar{\zeta}_1, \dots, \bar{\zeta}_N$ generators of $\Lambda(V)$.

Integration form: $\prod_{\mu=1}^{N} \frac{\partial^2}{\partial \zeta^\mu \partial \bar{\zeta}_\mu}$.

Express linear operator $B \in \mathrm{End}(V) \simeq V \otimes V^*$ as $B = \sum_{\mu\nu} B^\mu{}_\nu \, e_\mu \otimes e^\nu$.

<u>CLAIM.</u> $\int_\zeta \exp\left(\sum_{\mu\nu} B^\mu{}_\nu \bar{\zeta}_\mu \zeta^\nu \right) = \mathrm{Det}(B)$.

<u>Proof.</u>
$$\int_\zeta \exp\left(\sum_{\mu\nu} B^\mu{}_\nu \bar{\zeta}_\mu \zeta^\nu \right) = \frac{1}{N!} \int_\zeta \left(\sum_{\mu\nu} B^\mu{}_\nu \bar{\zeta}_\mu \zeta^\nu \right)^N =$$
$$= \frac{1}{N!} \int_\zeta \sum_{\pi, \pi' \in S_N} B^{\pi(1)}{}_{\pi'(1)} \bar{\zeta}_{\pi(1)} \zeta^{\pi'(1)} \cdots B^{\pi(N)}{}_{\pi'(N)} \bar{\zeta}_{\pi(N)} \zeta^{\pi'(N)}$$
$$= \frac{1}{N!} \int_\zeta \sum_{\pi, \pi' \in S_N} \mathrm{sgn}(\pi)\, \mathrm{sgn}(\pi')\, B^{\pi(1)}{}_{\pi'(1)} \cdots B^{\pi(N)}{}_{\pi'(N)} = \sum_{\pi \in S_N} \mathrm{sgn}(\pi) B^{\pi(1)}{}_1 \cdots B^{\pi(N)}{}_N$$
$$= \mathrm{Det}(B). \blacksquare$$

Pfaffian from Gaussian Berezin integral — "real" version.

Let $A : W \otimes W \to \mathbb{C}$ be a skew-symmetric bilinear form; $\dim W = N$.

Express A in a basis $\{e_\mu\}$ of W (with dual basis $\{e^\mu\}$) by
$$A = \sum_{\mu,\nu} A_{\mu\nu} \, e^\mu \otimes e^\nu \quad \text{where} \quad A_{\mu\nu} = A(e_\mu, e_\nu) = -A_{\nu\mu}.$$

Choose the Berezin integration form given by the ordered basis $e_1, \dots, e_N$ ($e^\mu \equiv \xi^\mu$):
$$f \in \Lambda(W^*) \mapsto \int_\xi f := \frac{\partial^N}{\partial \xi^N \cdots \partial \xi^2 \partial \xi^1} f.$$

Definition (Pfaffian). $\mathrm{Pf}(A) := \int_\xi \exp\left(\frac{1}{2} \sum_{\mu\nu} A_{\mu\nu} \xi^\mu \xi^\nu \right)$.

<u>Examples.</u> N odd $\rightsquigarrow \mathrm{Pf}(A) \equiv 0$, $\quad N = 2 : \mathrm{Pf}(A) = A_{12}$,
$N = 4 : \mathrm{Pf}(A) = A_{12} A_{34} - A_{13} A_{24} + A_{14} A_{23}$.

<u>Info.</u> The determinant of a skew-symmetric matrix has an analytic square root, namely the Pfaffian: $\mathrm{Pf}(A) = \pm \sqrt{\mathrm{Det}(A)}$.

IV.7 Derivation of path integral

Motivation. Express the relevant objects of quantum statistical physics of interacting fermions (grand canonical partition function, etc.) as (functional) integrals.

Let $V = \mathbb{C}^N$ and $W = V \oplus V^*$.

Clifford algebra $Cl(W)$ with generators c_i^+, c_i.

Grassmann algebra $\Lambda(W)$ with generators $\bar\zeta_i, \zeta_i$.

Consider the operator $T_\zeta := \exp\left(\sum_j c_j^+ \zeta_j - \sum_j \bar\zeta_j c_j\right)$.

<u>Convention</u> (Koszul sign rule): Clifford and Grassmann generators anticommute with each other, i.e., $c_i^+ \zeta_j = -\zeta_j c_i^+$ etc.

Fact. By using the algebraic relations for the Clifford and Grassmann generators, one deduces the multiplication law

$$T_\zeta T_{\zeta'} = T_{\zeta+\zeta'}\, e^{-\frac{1}{2}\sum_j (\bar\zeta_j \zeta'_j + \zeta_j \bar\zeta'_j)}.$$

<u>Remark</u>. To prove this relation, one uses the BCH series

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\dots}$$

In the present instance the series terminates at the first commutator term. To compute the commutator, one observes that our convention (see above) turns it into the <u>anticommutator</u> for the Fock operators. For example:

$$\left[\sum_i c_i^+\zeta_i , \sum_j \bar\zeta_j c_j\right] = \sum_{ij}\left(c_i^+\zeta_i\bar\zeta_j c_j - \bar\zeta_j c_j c_i^+ \zeta_i\right)$$
$$= \sum_{ij} \zeta_i\left(c_i^+ c_j + c_j c_i^+\right)\bar\zeta_j = \sum_i \zeta_i \bar\zeta_i .$$

Let $\Pi_0 = |0\rangle\langle 0|$ denote the projector on the Fock vacuum.

Lemma. $\mathrm{Id}_{\Lambda(V)} = \int d^N\bar\zeta\, d^N\zeta\; T_\zeta\, \Pi_0\, T_\zeta^{-1}$.

Proof for $N = 1$ (by direct calculation):

$$\int d\bar\zeta\, d\zeta\; T_\zeta \Pi_0 T_\zeta^{-1} = \int d\bar\zeta\, d\zeta \left(1 + c^+\zeta - \tfrac{1}{2}\bar\zeta c c^+ \zeta\right) |0\rangle\langle 0| \left(1 + \bar\zeta c - \tfrac{1}{2}\bar\zeta c c^+ \zeta\right)$$
$$= \frac{\partial}{\partial\bar\zeta}\frac{\partial}{\partial\zeta}\left(-\tfrac{1}{2}\bar\zeta\zeta\, c c^+ |0\rangle\langle 0| - \tfrac{1}{2}\bar\zeta\zeta\, |0\rangle\langle 0| c c^+ + \zeta\bar\zeta\, c^+|0\rangle\langle 0| c\right)$$
$$= |0\rangle\langle 0| + |1\rangle\langle 1| = \mathrm{Id}_{\Lambda(V)}\,. \checkmark$$

Conceptual proof.

To prove the Lemma for higher values of N we use the following foundational facts.

1. The Clifford algebra $\mathrm{Cl}(V \oplus V^*)$ acts irreducibly on the Fock space $\wedge(V)$.

   [Info: "Irreducible" means that there exists no subspace $\mathcal{U} \subset \wedge(V)$ which is invariant $\left(\mathrm{Cl}(V \oplus V^*)\, \mathcal{U} \subset \mathcal{U}\right)$ and proper $\left(\mathcal{U} \neq 0 \text{ and } \mathcal{U} \neq \wedge(V)\right)$.]

2. Schur's Lemma: Let a group G act irreducibly on a finite-dimensional representation space $\mathcal{V}$. Then if an endomorphism $X \in \mathrm{End}(\mathcal{V})$ commutes with the action of all group elements $g \in G$ on $\mathcal{V}$, that endomorphism must be a scalar multiple of the identity: $X = \text{const} \cdot \mathrm{Id}_{\mathcal{V}}$. [Warning: Schur's Lemma holds over the algebraically complete field $\mathbb{C}$. (It may fail over $\mathbb{R}$.)]

3. In view of the above, we consider the commutator of $X = \int d^N\bar{\zeta}\, d^N\zeta \; T_\zeta \Pi_0 T_\zeta^{-1}$ with any operator $T_{\zeta'}$ and show that it vanishes:

   $$T_{\zeta'} X = \int d^N\bar{\zeta}\, d^N\zeta \; T_{\zeta'} T_\zeta \Pi_0 T_\zeta^{-1} = \int d^N\bar{\zeta}\, d^N\zeta \; T_{\zeta'+\zeta} \Pi_0 T_\zeta^{-1} \; e^{-\frac{1}{2}\omega(\zeta',\zeta)} \quad \text{where}$$

   $$\omega(\zeta',\zeta) = \sum_j \left(\bar{\zeta}_j' \zeta_j + \zeta_j' \bar{\zeta}_j \right) = -\,\omega(\zeta,\zeta') \quad \text{is skew.}$$

   By the variable substitution $\zeta \longrightarrow \zeta - \zeta'$ one gets

   $$T_{\zeta'} X = \int d^N\bar{\zeta}\, d^N\zeta \; T_\zeta \Pi_0 T_{\zeta-\zeta'}^{-1} \; e^{-\frac{1}{2}\omega(\zeta',\zeta-\zeta')}.$$

   Now $T_{\zeta-\zeta'}^{-1} = \left(T_{-\zeta'} T_\zeta \, e^{\frac{1}{2}\omega(-\zeta',\zeta)} \right)^{-1} = T_\zeta^{-1} \, T_{-\zeta'}^{-1} \; e^{\frac{1}{2}\omega(\zeta',\zeta)}$.

   Hence $T_{\zeta'} X = \int d^N\bar{\zeta}\, d^N\zeta \; T_\zeta \Pi_0 T_\zeta^{-1} T_{-\zeta'}^{-1} \; e^{\frac{1}{2}\omega(\zeta',\zeta)} e^{-\frac{1}{2}\omega(\zeta',\zeta)} = X T_{\zeta'}$.

4. By the linear independence of the Grassmann variables ζ_j and $\bar{\zeta}_j$ it follows that X commutes with every Clifford generator c_j^+ and c_j. An adaptation of Schur's Lemma to the present setting then completes the proof of $X \propto \mathrm{Id}_{\wedge(V)}$.

   The constant of proportionality is determined easily by computing $\langle \mathrm{vac} | X | \mathrm{vac} \rangle = 1$.

Two Formulas: 1. $c_j T_\zeta \Pi_0 = \zeta_j T_\zeta \Pi_0$,

2. $\Pi_0 T_\zeta^{-1} c_j^+ = \Pi_0 T_\zeta^{-1} \bar\zeta_j$.

Proof of the second formula. Write $\Pi_0 T_\zeta^{-1} c_i^+ = \Pi_0 \left(T_\zeta^{-1} c_i^+ T_\zeta\right) T_\zeta^{-1}$.

$$T_\zeta^{-1} c_j^+ T_\zeta = e^{-\left[\sum_j c_j^+ \zeta_j - \sum_j \bar\zeta_j c_j \,,\, \cdot\,\right]} c_i^+ = c_i^+ - \left[\sum_j c_j^+ \zeta_j - \sum_j \bar\zeta_j c_j \,,\, c_i^+\right] + 0$$

$$= c_i^+ + \sum_j \left[\bar\zeta_j c_j \,,\, c_i^+\right] = c_i^+ + \sum_j \bar\zeta_j \left(c_j c_i^+ + c_i^+ c_j\right) = c_i^+ + \bar\zeta_i \,,$$

$$\text{so} \quad \Pi_0 T_\zeta^{-1} c_i^+ = \Pi_0 \left(c_i^+ + \bar\zeta_i\right) T_\zeta^{-1} = \Pi_0 T_\zeta^{-1} \bar\zeta_i \,.$$

Derivation of the functional integral.

$$\mathrm{Tr}\, e^{-\beta \hat H} = \mathrm{Tr}\left(\mathrm{Id}_{\Lambda(V)}\, e^{-\frac12 \beta \hat H}\, \mathrm{Id}_{\Lambda(V)}\, e^{-\frac12 \beta \hat H}\right)$$

$$= \int d^N\bar\zeta\, d^N\zeta \int d^N\bar\zeta' d^N\zeta' \;\mathrm{Tr}\left(T_\zeta \Pi_0 T_\zeta^{-1} e^{-\frac12 \beta \hat H}\, T_{\zeta'} \Pi_0 T_{\zeta'}^{-1} e^{-\frac12 \beta \hat H}\right).$$

Warning:

$\mathrm{Tr}(T_\zeta R) \overset{?}{=} \mathrm{Tr}(R T_\zeta)$ does not hold here! The correct identity is

$\mathrm{Tr}(T_\zeta R) \overset{\checkmark}{=} \mathrm{Tr}(R T_{-\zeta})$. This seen as follows.

Decompose $T_\zeta = (T_\zeta)_{\text{even}} + (T_\zeta)_{\text{odd}}$, $R = R_{\text{even}} + R_{\text{odd}}$ (with respect to fermion number parity) and notice that both $(T_\zeta)_{\text{odd}}$ and R_{odd} are odd in the number of Clifford generators as well as in the number of Grassmann variables. Now

$$\mathrm{Tr}(T_\zeta R) = \mathrm{Tr}\left((T_\zeta)_{\text{even}} R_{\text{even}}\right) + \mathrm{Tr}\left((T_\zeta)_{\text{odd}} R_{\text{odd}}\right)$$

$$= \mathrm{Tr}\left(R_{\text{even}} (T_\zeta)_{\text{even}}\right) - \mathrm{Tr}\left(R_{\text{odd}} (T_\zeta)_{\text{odd}}\right)$$

$$= \mathrm{Tr}\left(R_{\text{even}} (T_{-\zeta})_{\text{even}}\right) + \mathrm{Tr}\left(R_{\text{odd}} (T_{-\zeta})_{\text{odd}}\right) = \mathrm{Tr}\left(R T_{-\zeta}\right).$$

The sign change in the second equality is caused by the transposition of Grassmann variables. (For the Clifford generators one has relations such as $\mathrm{Tr}(c^+ c) = \mathrm{Tr}(c c^+)$.)

Continue the derivation of the functional integral:

$$\mathrm{Tr}\, e^{-\beta \hat H} = \int d^N\bar\zeta\, d^N\zeta \int d^N\bar\zeta' d^N\zeta' \;\mathrm{Tr}\left(\Pi_0 T_\zeta^{-1} e^{-\frac12 \beta \hat H}\, T_{\zeta'} \Pi_0^2 T_{\zeta'}^{-1} e^{-\frac12 \beta \hat H}\, T_{-\zeta} \Pi_0\right).$$

The essential building block is $\Pi_0 T_\zeta^{-1} e^{-\frac12 \beta \hat H} T_{\zeta'} \Pi_0$.

For a large number M of imaginary-time discretization steps we have

$$\Pi_0 T_\zeta^{-1} e^{-\frac{1}{M}\beta\hat{H}} T_{\zeta'}\Pi_0 = \Pi_0 T_\zeta^{-1}\left(1-\tfrac{1}{M}\beta\hat{H}+\dots\right) T_{\zeta'}\Pi_0 .$$

Now we normal-order $\hat{H}$ (i.e. creation operators are moved to the left, annihilation operators to the right: $\hat{H} \equiv \hat{H}(c^+,c)$) and use the formulas 1 & 2 above, i.e. we substitute $c^+ \to \bar{\zeta}$ and $c \to \zeta'$. Then

$$\Pi_0 T_\zeta^{-1} e^{-\frac{1}{M}\beta\hat{H}} T_{\zeta'}\Pi_0 = \Pi_0 T_\zeta^{-1}\left(1-\tfrac{1}{M}\beta \hat{H}(c^+,c)+\dots\right) T_{\zeta'}\Pi_0$$

$$= \Pi_0 T_\zeta^{-1}\left(1-\tfrac{1}{M}\beta H(\bar{\zeta},\zeta')+\dots\right) T_{\zeta'}\Pi_0 \approx e^{-\frac{1}{M}\beta H(\bar{\zeta},\zeta')}\,\Pi_0 T_\zeta^{-1} T_{\zeta'}\Pi_0 .$$

Now we calculate $\Pi_0 T_\zeta^{-1} T_{\zeta'}\Pi_0 = \Pi_0 T_{-\zeta} T_{\zeta'}\Pi_0 = \Pi_0 T_{-\zeta} T_{\zeta'}\Pi_0\, e^{\frac{1}{2}(\bar{\zeta}\zeta'+\zeta\bar{\zeta}')}$

$$\dots = \Pi_0\, e^{-\frac{1}{2}(\bar{\zeta}'-\bar{\zeta})(\zeta'-\zeta)}\, e^{\frac{1}{2}(\bar{\zeta}\zeta'-\bar{\zeta}'\zeta)} = \Pi_0\, e^{\bar{\zeta}\zeta'-\frac{1}{2}\bar{\zeta}\zeta-\frac{1}{2}\bar{\zeta}'\zeta'} .$$

Thus our building block becomes (in the limit of large M)

$$\Pi_0 T_\zeta^{-1} e^{-\frac{1}{M}\beta\hat{H}} T_{\zeta'}\Pi_0 = \Pi_0\, e^{\bar{\zeta}\zeta'-\frac{1}{2}\bar{\zeta}\zeta-\frac{1}{2}\bar{\zeta}'\zeta'-\frac{1}{M}\beta H(\bar{\zeta},\zeta')} .$$

Taking into account the sign change in the last factor, we conclude that

$$\mathrm{Tr}\, e^{-\beta\hat{H}} = \lim_{M\to\infty} \int d^N\bar{\zeta}_1 d^N\zeta_1 \cdots \int d^N\bar{\zeta}_M d^N\zeta_M$$
$$\exp\sum_{k=2}^{M}\left(\bar{\zeta}_k\zeta_{k-1}-\tfrac{1}{2}\bar{\zeta}_k\zeta_k-\tfrac{1}{2}\bar{\zeta}_{k-1}\zeta_{k-1}-\tfrac{\beta}{M}H(\bar{\zeta}_k,\zeta_{k-1})\right)$$
$$\exp\left(\bar{\zeta}_1(-\zeta_M)-\tfrac{1}{2}\bar{\zeta}_1\zeta_1-\tfrac{1}{2}(-\bar{\zeta}_M)(-\zeta_M)-\tfrac{\beta}{M}H(\bar{\zeta}_1,-\zeta_M)\right).$$

Assuming the continuum limit (justification?!) and changing notation $\zeta \to \psi$, $\bar{\zeta} \to \bar{\psi}$, one writes the result in the form

$$\mathrm{Tr}\, e^{-\beta\hat{H}} = \int \mathcal{D}[\psi(\tau)]\; e^{-\oint_0^\beta d\tau\,\left(\bar{\psi}\frac{\partial}{\partial\tau}\psi + H(\bar{\psi},\psi)\right)}$$

with anti-periodic boundary conditions $\psi(\beta) = -\psi(0)$, $\bar{\psi}(\beta) = -\bar{\psi}(0)$.

Transcription. Time evolution trace:

$$\mathrm{Tr}\, e^{-it\hat{H}/\hbar} = \int \mathcal{D}[\psi(t)]\; e^{\frac{i}{\hbar}\oint_0^T dt\,\left(i\hbar\bar{\psi}\frac{\partial}{\partial t}\psi - H(\bar{\psi},\psi)\right)} .$$

Exercise. Given the free Dirac Hamiltonian $\hat{H}_0$ show that the time evolution trace is $\mathrm{Tr}\, e^{-it\hat{H}_0/\hbar} = \int \mathcal{D}\psi\; e^{\frac{i}{\hbar}S_{\mathrm{Dirac}}}$ with

$$S_{\mathrm{Dirac}} = \int d^4x\; \bar{\psi}\left(i\hbar\gamma^\mu\frac{\partial}{\partial x^\mu} - mc\right)\psi .$$

Charge conjugation 'mystery' resolved.

i. First-quantized theory. $\psi \mapsto C\psi = \beta\alpha_2\bar{\psi}$ (complex antilinear),

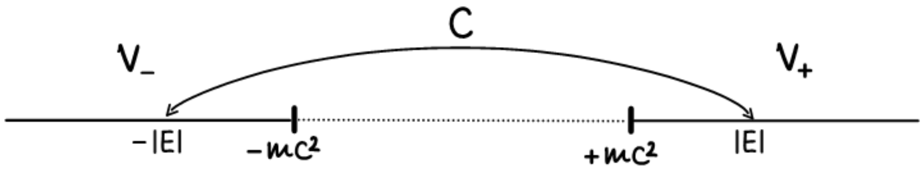
$$C\,H(\phi,\vec{A})\,C^{-1} = -H(-\phi,-\vec{A}).$$

Let $H(0,0) \equiv H_0$.

$$CH_0 = -H_0C \implies CV_+ = V_- \text{ and } CV_- = V_+ .$$

Notice $i\hbar\frac{\partial}{\partial t}\psi = H(\phi,\vec{A})\psi \implies i\hbar\frac{\partial}{\partial t}\psi^c = H(-\phi,-\vec{A})\psi^c,$

$$\psi^c = C\psi.$$



ii. Second-quantized theory.

$$\hat{C}:\quad \Lambda(V_+\otimes V_-^*) \xrightarrow[\text{antilinear}]{C} \Lambda(V_-\otimes V_+^*) \xrightarrow[\text{antilinear}]{|\,\rangle \overset{FR}{\longleftrightarrow} \langle\,|} \Lambda(V_+\otimes V_-^*) \quad \text{linear map.}$$

Remark. electron$(\hbar\omega,\hbar k,\hbar s) \overset{\hat{C}}{\longleftrightarrow}$ positron$(\hbar\omega,\hbar k,\hbar s)$.

Summary (as a diagram).

$$\begin{tikzcd}
\psi = \arrow[ddd, leftrightarrow, bend right, "\mathrm{FR}"'] & \text{positive-energy spinor} \arrow[d, "\iota"] \arrow[rr, leftrightarrow, bend left, "C \equiv C_{\text{class}}"] & + & \text{negative-energy spinor} \arrow[d, "\varepsilon"] \arrow[ddd, leftrightarrow, bend left, "\mathrm{FR}"] \\
& \text{annihilates electron} \arrow[rrd, leftrightarrow, "\hat{C} \equiv C_{\text{quant}}"] & & \text{creates positron} \arrow[lld, leftrightarrow, "\hat{C} \equiv C_{\text{quant}}"'] \\
& \text{creates electron} & & \text{annihilates positron} \\
\tilde{\psi} = & \text{positive-energy co-spinor} \arrow[u, "\varepsilon"] \arrow[rr, leftrightarrow, bend right, "C \equiv C_{\text{class}}"'] & + & \text{negative-energy co-spinor} \arrow[u, "\iota"]
\end{tikzcd}$$

IV.8 Spinor representation of the Lorentz group

Under a Lorentz transformation $g \in SO(1,3)$ (= Lorentz group)

- a scalar field $\varphi : \mathbb{R}^4 \to \mathbb{C}$ transforms as $(g\cdot\varphi)(v) = \varphi(g^{-1}v)$;
- a vector field $A : \mathbb{R}^4 \to \mathbb{R}^4$ transforms as $(g\cdot A)(v) = g\, A(g^{-1}v)$;
- a spinor field $\psi : \mathbb{R}^4 \to \mathbb{C}^4$ transforms as $(g\cdot\psi)(v) = S(g)\,\psi(g^{-1}v)$.

Here $g \mapsto S(g)$ is a projective representation called the spinor representation of $SO(1,3)$. It is defined as follows.

1. Write $g = e^X$ (note that X is not uniquely defined, as the exponential map has a non-trivial kernel on Lie $SO(1,3)$).
2. Convert the linear transformation $X : \mathbb{R}^4 \to \mathbb{R}^4$ into a skew-symmetric bilinear form $\tilde{X} : \mathbb{R}^4 \times \mathbb{R}^4 \to \mathbb{R}$ by means of the Minkowski metric Q: $\tilde{X}(u,v) = Q(Xu, v)$. In components: $\tilde{X}_{\mu\nu} = Q_{\mu\lambda} X^\lambda{}_\nu$.
3. Given a choice of gamma matrices put $S(e^X) = \exp\left(-\frac{1}{8}\tilde{X}_{\mu\nu}[\gamma^\mu, \gamma^\nu]\right)$
$$= \exp\left(-\tfrac{1}{4} X^\mu{}_\nu\, \gamma_\mu \gamma^\nu\right).$$

Fact. If a spinor field $v \mapsto \psi(v)$ satisfies the Dirac equation, then so does the Lorentz-transformed spinor field $v \mapsto S(g)\,\psi(g^{-1}v)$.

<u>Remark</u>. This comes about because under Lorentz transformations $g \in SO(1,3)$ one has

$$\underset{\text{vector repn of } SO(1,3)}{\frac{\partial}{\partial x^\mu} \mapsto \frac{\partial}{\partial x^\nu}\, g^\nu{}_\mu} \quad \text{and} \quad \underset{\text{co-vector repn of } SO(3,1)}{\gamma^\mu \mapsto S(g)\,\gamma^\mu S(g)^{-1} = (g^{-1})^\mu{}_\nu\, \gamma^\nu}$$

so that $\gamma^\mu \frac{\partial}{\partial x^\mu}$ is invariant.

Info. The spinor represention $g \mapsto S(g)$ is projective due to a sign ambiguity: $S(g_1)S(g_2) = \pm S(g_1 g_2)$. It lifts to a true representation of Spin(1,3), a 2:1 cover of $SO(1,3)$.

Pseudo-unitarity. $S(g)^\dagger = e^{-\frac{1}{8}\tilde{X}_{\mu\nu}[\gamma^{\nu\dagger}, \gamma^{\mu\dagger}]} \overset{\gamma^{\mu\dagger} = \gamma^0\gamma^\mu\gamma^0}{=} e^{\frac{1}{8}\tilde{X}_{\mu\nu}\gamma^0[\gamma^\mu,\gamma^\nu]\gamma^0} = \gamma^0 S(g)^{-1}\gamma^0.$

<u>Note</u>. It follows that $\bar{\psi}\psi \equiv \psi^\dagger\gamma^0\psi$ transforms as a Lorentz scalar. [The charge density function $\rho = e\bar{\psi}\gamma^0\psi = e\psi^\dagger\psi$ transforms as the time-component of the charge-current Lorentz vector $J^\mu = e\bar{\psi}\gamma^\mu\psi$.]

Application: Covariantly normalized H_0-eigenspinors.

$k_\mu = (-\omega/c, \vec{k})$

Insert the plane-wave ansatz $\psi = e^{i(k\cdot r - \omega t)} u_s(k) \equiv e^{ik_\mu x^\mu} u_s(k)$ into the covariant form of the Dirac equation. Then $\left(\gamma^\mu k_\mu + \frac{mc}{\hbar}\right) u_s(k) = 0$. To solve this equation, one starts from the rest frame where momentum $\hbar k = 0$ and energy $\hbar\omega = mc^2$, and one sets

$$u_\uparrow(0) = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad u_\downarrow(0) = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \quad v_\downarrow(0) = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad v_\uparrow(0) = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

It is immediately clear that these are solutions for $k_\mu = k_\mu^{(\text{rest})} = (-mc/\hbar, \vec{0})$ (u), resp. $k_\mu = k_\mu^{(\text{rest})} = (+mc/\hbar, \vec{0})$ (v). To obtain solutions for any k_μ, one applies a Lorentz boost $g(k)$ transforming $k_\mu^{(\text{rest})}$ into the actual k_μ. By the construction of the spinor representation one has $S(g(k))\, \gamma^\mu k_\mu^{(\text{rest})}\, S(g(k))^{-1} = \gamma^\mu k_\mu$. Hence $u_s(k) = S(g(k))\, u_s(0)$ and $v_s(k) = S(g(k))\, v_s(0)$ are solutions.

<u>Note</u>. By the pseudo-unitarity relation for $S(g)$ one has

$$u_s(k)^\dagger \gamma^0 u_{s'}(k) = u_s(0)^\dagger S(g(k))^\dagger \gamma^0 S(g(k))\, u_{s'}(0) = u_s(0)^\dagger \gamma^0 u_{s'}(0) = \delta_{ss'}$$

and $v_s(k)^\dagger \gamma^0 v_{s'}(k) = v_s(0)^\dagger S(g(k))^\dagger \gamma^0 S(g(k))\, v_{s'}(0) = v_s(0)^\dagger \gamma^0 v_{s'}(0) = -\delta_{ss'}$.

Remark ($\longrightarrow$ spinor representation of the rotation group SO(3)).

- orbital angular momentum L: phase space $\xrightarrow{\text{equivariant}}$ Lie SO(3) (math: "moment map"),

$$L = (x^k p_\ell - p^k x_\ell)\, e_k \otimes f^\ell = x^k p_\ell\,(e_k \otimes f^\ell - e^\ell \otimes f_k).$$

- spin angular momentum S: spinor space $\xrightarrow{\text{eqvt}}$ Lie SO(3).

Warning — change of notation: $g \in SU(2)$, $R \in SO(3)$.

$$S:\ \psi \longmapsto \frac{i\hbar}{4}\langle\psi|[\sigma^k,\sigma_\ell]|\psi\rangle\, e_k \otimes f^\ell, \qquad \psi \in \mathbb{C}^2.$$

S equivariant means that SO(3) acts on the domain and the range of S and the effect of the action is the same:

$$\langle g\psi|[\sigma^k,\sigma_\ell]|g\psi\rangle\, e_k \otimes f^\ell = \langle\psi|[\sigma^k,\sigma_\ell]|\psi\rangle\, Re_k \otimes f^\ell \circ R^{-1}.$$

Now $Re_k = e_{k'} R^{k'}{}_k$ and $f^\ell \circ R^{-1} = (R^{-1})^\ell{}_{\ell'} f^{\ell'}$.

Hence, the equivariance of S implies that $g^\dagger \sigma^k g = R^k{}_{k'}\sigma^{k'}$ and $g^\dagger \sigma_\ell\, g = \sigma_{\ell'} (R^{-1})^{\ell'}{}_\ell$ or, in final form, $\boxed{g\,\sigma_\ell\, g^{-1} = \sigma_{\ell'} R^{\ell'}{}_\ell}$.

This can be read in two ways. (i) Given $g \in SU(2)$, one finds $R \in SO(3)$ from the relation in the box. This gives a mapping $SU(2) \ni g \longmapsto R(g) \in SO(3)$. Note that $R(g) = R(-g)$. Thus the mapping is 2:1, as one is "taking a square". (ii) Conversely, given $R \in SO(3)$ one may want to "take the square root" $S(R) := \pm g \longleftarrow R$. That's the spinor representation.

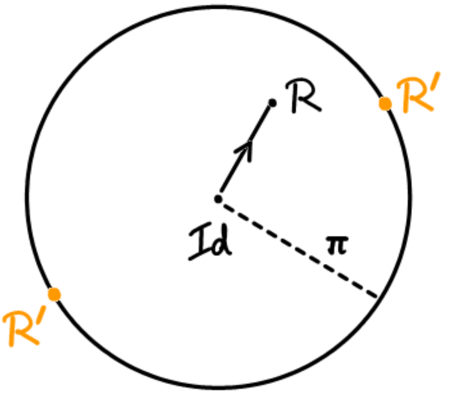
Notes. ① $SU(2) = \mathrm{Spin}(3)$ (accidental isomorphism).

② $SU(2) \ni g \longmapsto R(g) \in SO(3)$ generalizes to $\mathrm{Spin}(d) \ni g \longmapsto R(g) \in SO(d)$.

③ $\pi_1(SO(3)) = \mathbb{Z}_2$ and Spin(3) is the universal covering group of SO(3).

④ The relation in the box generalizes to $S(R)\,\gamma_\mu\, S(R)^{-1} = \gamma_\nu R^\nu{}_\mu$.

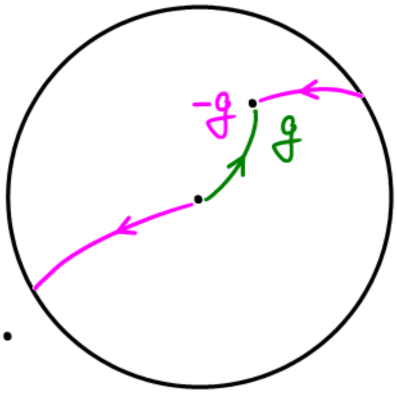
Added explanation for ③.



- Model for SO(3): a ball of radius π, where points on the surface of the ball are identified with their antipodal points.

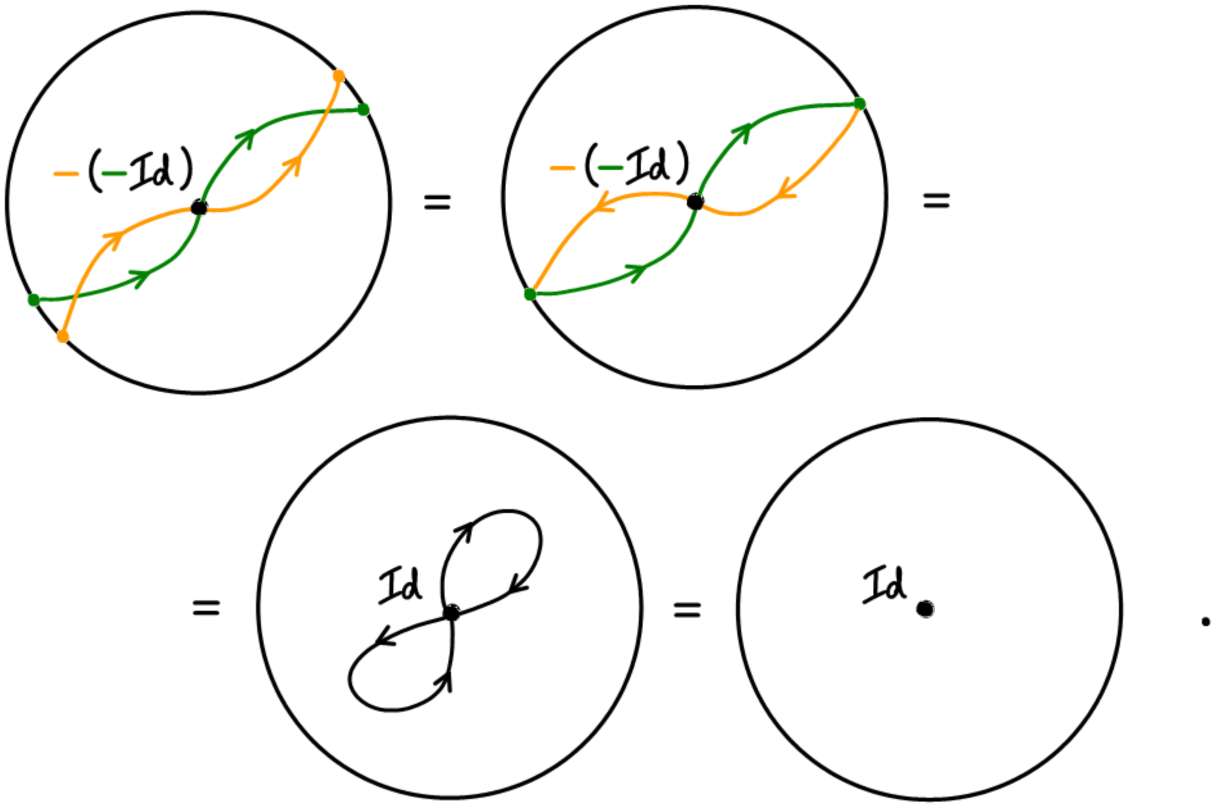
In this model, an element $R \in SO(3)$ is specified by its rotation axis (≙ straight line from Id to R) and a positive rotation angle (≙ distance between Id and R) & right-hand rule.

- Model for Spin(3) (by augmentation of the model for SO(3)):



An element $g \in \text{Spin}(3)$ is an element $R \in SO(3)$ in conjunction with a homotopy class of paths (continuously deformable "string") going from Id to R.

<u>Note</u>.



[Individually, the green and orange paths are non-contractible in SO(3) (they represent the nontrivial element in the fundamental group $\pi_1(SO(3)) = \mathbb{Z}_2$), but their simultaneous presence makes for a contractible path (as shown).]

IV.9 Feynman propagator.

In the perturbation expansion (interaction picture) for the scattering matrix we will encounter time-ordered products

$$\mathcal{T}\left(\psi^a(x)\,\bar\psi_b(y)\right) = \begin{cases} +\,\psi^a(x)\,\bar\psi_b(y) & \text{if } x^0 > y^0\,, \\ -\,\bar\psi_b(y)\,\psi^a(x) & \text{if } x^0 < y^0\,. \end{cases}$$

Time-ordered (or causal) one-particle Green's function ("propagator"):

$$G^a{}_b(x,y) = \langle \mathrm{vac} |\, \mathcal{T}\left(\psi^a(x)\,\bar\psi_b(y)\right) | \mathrm{vac} \rangle\,.$$

Recall the mode expansion (Warning: simplified notation $\hat\psi \equiv \psi$)

$$\psi^a(x) = \int \frac{d^3k}{(2\pi)^3}\sqrt{\frac{mc^2}{\hbar\omega(k)}}\sum_s \left(u_s(k)^a e^{+ik\cdot x}\,\iota(c_s^+(k)) + v_s(k)^a e^{-ik\cdot x}\,\varepsilon(c_s^-(k))\right),$$

$$\bar\psi_b(x) = \int \frac{d^3k}{(2\pi)^3}\sqrt{\frac{mc^2}{\hbar\omega(k)}}\sum_s \left(\varepsilon(\overline{c_s^+(k)})\, e^{-ik\cdot x}\,\bar u_s(k)_b + \iota(\overline{c_s^-(k)})\, e^{+ik\cdot x}\,\bar v_s(k)_b\right).$$

$$\Longrightarrow\ G^a{}_b(x,y) = \begin{cases} +\displaystyle\int \frac{d^3k}{(2\pi)^3}\frac{mc^2}{\hbar\omega(k)}\, e^{ik_\mu(x^\mu - y^\mu)} \sum_s u_s(k)^a\,\bar u_s(k)_b & \text{if } x^0 > y^0, \\ -\displaystyle\int \frac{d^3k}{(2\pi)^3}\frac{mc^2}{\hbar\omega(k)}\, e^{-ik_\mu(x^\mu - y^\mu)} \sum_s v_s(k)^a\,\bar v_s(k)_b & \text{if } x^0 < y^0. \end{cases}$$

Exercise.

$$\sum_s u_s(k)^a\,\bar u_s(k)_b = \tfrac12\left(1 - \gamma^\mu \frac{\hbar k_\mu}{mc}\right)^a{}_b\,,$$

$$\sum_s v_s(k)^a\,\bar v_s(k)_b = -\tfrac12\left(1 + \gamma^\mu \frac{\hbar k_\mu}{mc}\right)^a{}_b\,.$$

[Background.

On the notion of propagator: free Schrödinger particle (non-relativistic).

$$G(r,t;r',0) \equiv \langle r |\, e^{-itH_0/\hbar}\, | r' \rangle\, \Theta(t) \quad \xleftarrow{} \text{Heaviside function } \Theta(t) = \begin{cases} 1 & t>0\,, \\ 0 & t<0\,. \end{cases}$$

$$= \sqrt{\frac{m}{2\pi i\hbar t}}^{\,3}\, e^{+im\frac{(r-r')^2}{2t\hbar}}\,\Theta(t) = \int \frac{d^3k}{(2\pi)^3}\, e^{ik\cdot(r-r') - i\frac{\hbar k^2}{2m}t}\,\Theta(t)\,.$$

Now $$e^{-i\frac{\hbar k^2}{2m}t}\,\Theta(t) = i\int_{\mathbb{R}} \frac{d\omega}{2\pi}\,\frac{e^{-i\omega t}}{\omega + i\varepsilon - \hbar k^2/2m}\,.$$

Hence $$G(r,t;r',t') = i\int_{\mathbb{R}^4} \frac{d^3k\,d\omega}{(2\pi)^4}\,\frac{e^{ik\cdot(r-r') - i\omega(t-t')}}{\omega + i\varepsilon - \hbar k^2/2m}\,.\ ]$$

Goal: Show that the time-ordered one-particle Green's function $G^a{}_b(x,y)$, which is an object defined in the second-quantized theory, can be computed from the data of the first-quantized theory.

Let $D = \not{\partial} + imc/\hbar$ (where $\not{\partial} \equiv \gamma^\mu \frac{\partial}{\partial x^\mu}$) be the free Dirac operator.

Since the differential operator D has a kernel (given by the solution space of the free Dirac equation) its inverse or Green's function $D^{-1} = \tilde{G}$ is defined only up to the addition of terms in that very kernel. We are going to demonstrate that with the right choice of boundary condition ("causality") one has $\tilde{G} = G$.

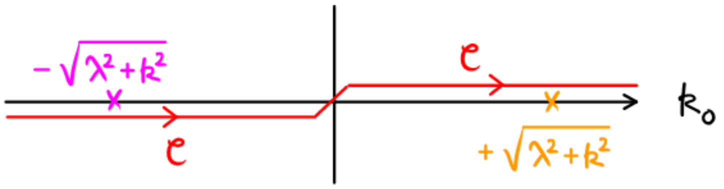
$$D^{-1} = \left(\not{\partial} - \tfrac{mc}{i\hbar}\right)^{-1} = \left(\not{\partial} - \tfrac{mc}{i\hbar}\right)^{-1}\left(\not{\partial} + \tfrac{mc}{i\hbar}\right)^{-1}\left(\not{\partial} + \tfrac{mc}{i\hbar}\right) = \left(\not{\partial}^2 + (mc/\hbar)^2\right)^{-1}\left(\not{\partial} + \tfrac{mc}{i\hbar}\right),$$

$$\text{so } (D^{-1})^a{}_b(x,y) = i\int \frac{d^4k}{(2\pi)^4}\, e^{ik_\mu(x-y)^\mu}\left(\frac{\not{k} - mc/\hbar}{-\not{k}^2 + (mc/\hbar)^2}\right)^a{}_b .$$

Now $\not{k}^2 = k_\mu\gamma^\mu k_\nu\gamma^\nu = \frac{1}{2}k_\mu k_\nu(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu) = k_0^2 - \vec{k}^2$. Hence

$$(D^{-1})^a{}_b(x,y) = i\int \frac{d^4k}{(2\pi)^4}\, e^{ik_\mu(x-y)^\mu}\, \frac{\not{k}^a{}_b - \lambda\delta^a{}_b}{-k_0^2 + \vec{k}^2 + \lambda^2} . \qquad \lambda = mc/\hbar$$

Choice of integration contour for k_0 (inner integration variable):



Then

$$(D^{-1})^a{}_b(x,y) = \begin{cases} \int \frac{d^3k}{(2\pi)^3}\frac{mc^2}{\hbar\omega(k)}\, e^{ik_\mu(x-y)^\mu}\, \frac{1}{2}\left(1 - \gamma^\mu \frac{\hbar k_\mu}{mc}\right)^a{}_b & \text{if } x^0 > y^0, \\ -\text{ same with } k_0 = -\omega(k)/c \longrightarrow k_0 = +\omega(k)/c & \text{if } x^0 < y^0. \end{cases}$$

Conclusion: $(D^{-1})^a{}_b(x,y) \overset{\checkmark}{=} G^a{}_b(x,y) = \langle \mathrm{vac} | T(\psi^a(x)\,\bar{\psi}_b(y)) | \mathrm{vac}\rangle$ for the choice $\mathcal{C}$ of energy integration contour.

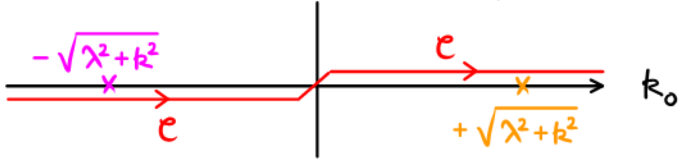
Stückelberg (1941): interpretation of positron as negative-energy electron traveling backward in time. Feynman (1947).

More on the path integral for the Dirac theory.

Recall the time-ordered one-particle Green's function:

$$\langle \mathrm{vac}|\mathcal{T}(\Psi^a(x)\bar{\Psi}_b(y))|\mathrm{vac}\rangle = G^a{}_b(x,y) \overset{!}{=} (D^{-1})^a{}_b(x,y), \quad D = \gamma^\mu\partial_\mu + imc/\hbar .$$

Feynman propagator D^{-1}



So far this (!) is just an observation. Accident? No! The relation follows directly from the fermionic path integral:

$$G^a{}_b(x,y) = \lim_{\varepsilon\to 0+} \lim_{T\to\infty\cdot e^{-i\varepsilon}} \frac{\mathrm{Tr}\, e^{-i\hat{H}T/2\hbar}\, \mathcal{T}(\Psi^a(x)\bar{\Psi}_b(y))\, e^{-i\hat{H}T/2\hbar}}{\mathrm{Tr}\, e^{-i\hat{H}T/\hbar}} .$$

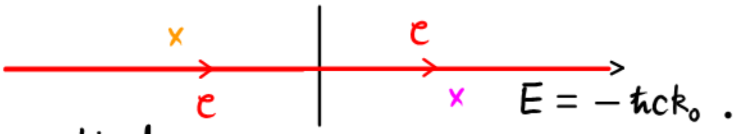
Since T occurs in the combination $\hat{H}T$, the factor $e^{-i\varepsilon}$ in T can be transferred to $\hat{H}$, thereby moving the eigenvalues of $\hat{H}$ (which are all positive but for the ground-state energy) into the lower half of the complex energy plane.

Use formulas 1. and 2. (from Lecture 22) to convert the operator $\mathcal{T}(\Psi^a(x)\bar{\Psi}_b(y))$ to a product $\psi^a(x)\bar{\psi}_b(y)$ of Grassmann variables. Then

$$G^a{}_b(x,y) = \lim_{T\to\infty} \frac{1}{Z_1} \int \partial\bar{\psi}\, \partial\psi\; e^{iS/\hbar}\, \psi^a(x)\bar{\psi}_b(y), \quad S = \int d^4x\, \bar{\psi}(\gamma^\mu\partial_\mu + i\tfrac{mc}{\hbar})\psi .$$

By carrying out the Gaussian Grassmann integral, one obtains

$G^a{}_b(x,y) \overset{\checkmark}{=} (D^{-1})^a{}_b(x,y)$, with the right-hand side (as a Fourier integral) given by the energy integration contour



Note that by returning from the second-quantized Hamiltonian $e^{-i\varepsilon}\hat{H}$ to the corresponding first-quantized Hamiltonian, the positron spectrum goes to the negative-energy axis and into the upper half of the complex-energy plane ($\curvearrowright$ Stückelberg: a positron is a negative-energy electron travelling backwards in time).

Note: the path integral always computes Green's functions that are time-ordered.

[Remark. A topic of study in current physics are out-of-time-order correlations (OTOC).]

IV.10 Wick's Theorem (correlation functions of a free theory).

So far our considerations have been based on $\mathrm{Tr}\, e^{-\beta(H-\mu n)}$ or $\mathrm{Tr}\, e^{-iTH/\hbar}$, but of more interest are, say, thermal expectation values; for example

$$\langle \text{local density} \rangle = \frac{1}{Z} \mathrm{Tr}\left(c^{+}(x)\, c(x)\; e^{-\beta(H-\mu n)}\right),$$

or dynamical correlation functions.

In preparation of the perturbation theory treatment of interacting systems we here consider free particles, which are described by a Gaussian functional integral with integrand $e^{-S[\bar{\psi},\psi]}$. We introduce the relevant tool (→ Wick's Theorem) in the discrete setting of $S = \bar{\zeta}_i A^i{}_j \zeta^j \equiv \bar{\zeta} A \zeta$.

Def (for $\mathrm{Det} A \neq 0$): $\quad \langle F(\zeta,\bar{\zeta}) \rangle \overset{\text{def}}{=} \dfrac{\int F(\zeta,\bar{\zeta})\, e^{-\bar{\zeta} A \zeta}}{\int e^{-\bar{\zeta} A \zeta}}, \quad \int \equiv \prod_{i=1}^{N} \dfrac{\partial^2}{\partial \bar{\zeta}_i \partial \zeta^i}$.

Sign convention $(N=1)$: $\int e^{-\bar{a}\zeta\zeta} = \dfrac{\partial^2}{\partial\bar{\zeta}\partial\zeta}(1 - a\bar{\zeta}\zeta) = a \dfrac{\partial^2}{\partial\bar{\zeta}\partial\zeta}\zeta\bar{\zeta} = a$.

⇝ Generalization: $\int e^{-\bar{\zeta} A \zeta} = \mathrm{Det}(A)$.

Fact (Wick's Theorem for complex fermions):

$$\left\langle \zeta^{j_1}\bar{\zeta}_{i_1}\, \zeta^{j_2}\bar{\zeta}_{i_2} \cdots \zeta^{j_n}\bar{\zeta}_{i_n} \right\rangle = \sum_{\pi \in S_n} \mathrm{sign}(\pi) \left\langle \zeta^{j_1}\bar{\zeta}_{i_{\pi(1)}} \right\rangle \left\langle \zeta^{j_2}\bar{\zeta}_{i_{\pi(2)}} \right\rangle \cdots \left\langle \zeta^{j_n}\bar{\zeta}_{i_{\pi(n)}} \right\rangle .$$

<u>Sketch of proof</u>. Consider the generating functional (with Grassmann variables $\eta, \bar{\eta}$ as "sources") $\quad Z[\eta,\bar{\eta}] := \int e^{-\bar{\zeta} A \zeta + \bar{\zeta}_i \eta^i + \bar{\eta}_i \zeta^i}$

$$= \int e^{-(\bar{\zeta} - \bar{\eta} A^{-1}) A (\zeta - A^{-1}\eta) + \bar{\eta} A^{-1} \eta}.$$

Now use the substitution rule (Berezin) with $\zeta - A^{-1}\eta = \zeta'$, $\bar{\zeta} - \bar{\eta} A^{-1} = \bar{\zeta}'$.

and $\int = \prod_i \dfrac{\partial^2}{\partial\bar{\zeta}_i \partial\zeta^i} = \prod_i \dfrac{\partial^2}{\partial\bar{\zeta}'_i \partial\zeta'^i}$ to obtain $Z[\eta,\bar{\eta}]/Z[0,\bar{0}] = e^{+\bar{\eta} A^{-1} \eta}$.

The desired result then follows by taking multiple derivatives with respect to $\eta, \bar{\eta}$ at zero:

$$\langle \zeta^j \bar{\zeta}_i \rangle = \frac{\partial^2}{\partial\eta^i \partial\bar{\eta}_j} \frac{Z[\eta,\bar{\eta}]}{Z[0,\bar{0}]}\bigg|_{\eta=\bar{\eta}=0} = \frac{\partial^2}{\partial\eta^i \partial\bar{\eta}_j} e^{\bar{\eta} A^{-1} \eta}\bigg|_{\eta=\bar{\eta}=0} = A^{-1\,j}{}_i ,$$

$$\langle \zeta^{j_1}\bar{\zeta}_{i_1}\, \zeta^{j_2}\bar{\zeta}_{i_2} \rangle = \frac{\partial^2}{\partial\eta^{i_1}\partial\bar{\eta}_{j_1}} \frac{\partial^2}{\partial\eta^{i_2}\partial\bar{\eta}_{j_2}} e^{\bar{\eta} A^{-1} \eta}\bigg|_{\eta=\bar{\eta}=0} = A^{-1\,j_1}{}_{i_1} A^{-1\,j_2}{}_{i_2} - A^{-1\,j_1}{}_{i_2} A^{-1\,j_2}{}_{i_1}, \text{ etc.}$$

Exercise. By using Wick's Theorem in the functional integral setting, derive a similar result in the operator setting, for $\langle X \rangle_0 \overset{\text{def}}{=} Z^{-1} \operatorname{Tr} X e^{-\beta(H-\mu n)}$. In particular, show that $\langle c_i^+ c^j c_k^+ c^\ell \rangle_0 = \langle c_i^+ c^j \rangle_0 \langle c_k^+ c^\ell \rangle_0 + \langle c_i^+ c_\ell \rangle_0 \langle c_j c_k^+ \rangle_0$.

Application. Density-density correlations in a free Fermi gas:

$$\langle \rho(x) \rho(y) \rangle_{\text{conn}} \equiv \langle \rho(x) \rho(y) \rangle_0 - \langle \rho(x) \rangle_0 \langle \rho(y) \rangle_0$$

$$= \langle c^+(x) c(x)\, c^+(y) c(y) \rangle_0 - \langle c^+(x) c(x) \rangle_0 \langle c^+(y) c(y) \rangle_0 = \langle c^+(x)\, c(y) \rangle_0 \langle c(x)\, c^+(y) \rangle_0 .$$

$$\langle c^+(x)\, c(y) \rangle_0 = \int \frac{d^d k}{(2\pi)^d}\, e^{ik(x-y)} \langle c_k^+ c^k \rangle_0 = \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik(x-y)}}{e^{\beta(\varepsilon_k - \mu)} + 1} ,$$

$$\langle c(x)\, c^+(y) \rangle_0 = \int \frac{d^d k}{(2\pi)^d}\, e^{-ik(x-y)} \langle c^k c_k^+ \rangle_0 = \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik(x-y)}}{e^{-\beta(\varepsilon_k - \mu)} + 1} .$$

$d=1$ and $\beta \to \infty$ $(T \to 0)$: $\langle c^+(x)\, c(y) \rangle_0 = \int_{-k_f}^{k_f} \frac{dk}{2\pi}\, e^{ik(x-y)} = \frac{\sin(k_f(x-y))}{\pi(x-y)}$,

$$\langle c(x)\, c^+(y) \rangle_0 = \int_{|k| > k_f} \frac{dk}{2\pi}\, e^{-ik(x-y)} = \delta(x-y) - \frac{\sin(k_f(x-y))}{\pi(x-y)} .$$

Hence

$$\langle \rho(x) \rho(y) \rangle_{\text{conn}} = \delta(x-y)\, \frac{k_f}{\pi} - \left(\frac{\sin(k_f(x-y))}{\pi(x-y)} \right)^2 \quad (\text{for } d=1 \text{ and } \beta \to \infty).$$

Appendix. How to remember $\langle \zeta^j \bar{\zeta}_i \rangle = A^{-1\,j}{}_i$.

$$\operatorname{Tr} \langle \zeta \bar{\zeta} \rangle\, \delta A = \langle -\bar{\zeta}\, \delta A \cdot \zeta \rangle = \operatorname{Det}^{-1}(A)\, \delta \int e^{-\bar{\zeta} A \zeta}$$

$$= \operatorname{Det}^{-1}(A)\, \delta \operatorname{Det}(A) = \operatorname{Tr} A^{-1} \delta A .$$

IV.11. Application: high-density electron gas.

Hamiltonian: $H-\mu N = \int d^3r\, \Psi^\dagger(r)\left(-\frac{\hbar^2}{2m}\Delta-\mu\right)\Psi(r)$

$$+\frac{1}{2}\int d^3r\int d^3r'\ \hat{\rho}(r)\,\frac{e^2}{4\pi\varepsilon_0|r-r'|}\,\hat{\rho}(r'), \qquad \hat{\rho}(r)=\Psi^\dagger(r)\Psi(r).$$

Grand canonical partition function: $Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \int \mathcal{D}\bar{\psi}\,\mathcal{D}\psi\ e^{-S}$,

$$S = \oint_0^\beta d\tau \left\{ \int d^3r\ \bar{\psi}(r,\tau)\left(\frac{\partial}{\partial\tau}-\frac{\hbar^2}{2m}\Delta-\mu\right)\psi(r,\tau) + \frac{1}{2}\int d^3r\int d^3r'\ \rho(r,\tau)\,\frac{e^2}{4\pi\varepsilon_0|r-r'|}\,\rho(r',\tau)\right\}.$$

Assume box $Q=[0,L]^3$ with periodic boundary conditions.

To take advantage of translation invariance, use Fourier transform:

$$\psi_{k\omega} = \oint_0^\beta d\tau \int_Q d^3r\ e^{-i(kr-\omega\tau)}\psi(r,\tau); \quad k\in\frac{2\pi}{L}\cdot\mathbb{Z}^3,\ \ \omega\in\frac{2\pi}{\beta}(\mathbb{Z}+1/2);$$

Inverse Fourier transform: $\psi(r,\tau) = \frac{1}{L^3\beta}\sum_{k\omega} e^{i(kr-\omega\tau)}\psi_{k\omega}$.

Adopt the convention $\bar{\psi}(r,\tau) = \frac{1}{L^3\beta}\sum_{k\omega} e^{-i(kr-\omega\tau)}\bar{\psi}_{k\omega}$.

Then $S = \frac{1}{L^3\beta}\sum_{k\omega}\left\{\bar{\psi}_{k\omega}\left(-i\omega+\frac{\hbar^2k^2}{2m}-\mu\right)\psi_{k\omega}+\frac{1}{2}\,\rho_{k\omega}\tilde{V}(k)\,\rho_{-k-\omega}\right\}$

where $\tilde{V}(k) = \frac{e^2}{\varepsilon_0|k|^2}$ Fourier transform of Coulomb potential.

Note: Coulomb potential $\notin L^1(\mathbb{R}^3)$ $\rightsquigarrow$ singularity at $k=0$. However, $k=0$ is dropped on physical grounds (overall charge neutrality).

Next. Introduce auxiliary field ϕ by generalization of the identity

$$e^{-\frac{a}{2}y^2} = \int_{\mathbb{R}}\frac{dx}{\sqrt{2\pi}}\,e^{-\frac{x^2}{2a}+ixy}.$$

Auxiliary-field treatment (Hubbard–Stratonovich transformation).

$$e^{-\frac{1}{2L^3\beta}\sum_{k\omega}\rho_{k\omega}\tilde{V}(k)\rho_{-k-\omega}}$$

Note $k\neq 0$ and $\rho_{0\omega}=0$ (← overall charge neutrality)

$$=\int\mathcal{D}\phi\ e^{-\frac{1}{L^3\beta}\sum_{k\omega}\left(\frac{e^2}{2}\phi_{k\omega}\tilde{V}(k)^{-1}\phi_{-k-\omega}+ie\,\phi_{k\omega}\,\rho_{-k-\omega}\right)}$$

where $\phi_{-k-\omega} = \overline{\phi}_{k\omega}$ (due to $\phi(r,\tau)$ real; see below),

$$\begin{aligned}\rho_{k\omega} &= \int d\tau \int d^3r\, e^{-i(kr-\omega\tau)}\, \overline{\psi}(r,\tau)\psi(r,\tau) \\ &= \frac{1}{L^3\beta} \sum_{k_1-k_2=k} \sum_{\omega_1-\omega_2=\omega} \overline{\psi}_{k_2\omega_2}\psi_{k_1\omega_1}.\end{aligned}$$

Extended action functional:

$$S_{\text{ext}}[\overline{\psi},\psi;\phi] = \frac{e^2}{2L^3\beta}\sum_{k\omega} |\phi_{k\omega}|^2\ \tilde{V}(k)^{-1}$$

$$+ \frac{1}{L^3\beta}\sum_{kk'\omega\omega'} \overline{\psi}_{k\omega}\left(\left(-i\omega + \frac{\hbar^2k^2}{2m} - \mu\right)\delta_{kk'}\,\delta_{\omega\omega'} + ie\,\phi_{k-k',\,\omega-\omega'}\right)\psi_{k'\omega'}.$$

Inverse Fourier transform $\leadsto$ $\phi_{k\omega} = \oint_0^\beta d\tau \int_Q d^3r\, e^{-i(kr-\omega\tau)}\phi(r,\tau)$.

Action in real space & imaginary time:

$$S_{\text{ext}}[\overline{\psi},\psi;\phi] = \oint_0^\beta d\tau \int_Q d^3r \left\{\frac{\varepsilon_0}{2}(\nabla\phi)^2 + \overline{\psi}\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right)\psi\right\}.$$

Remark. If one writes $-\nabla\phi = E$, then $\frac{\varepsilon_0}{2}\int d^3r\,(\nabla\phi)^2 = \frac{\varepsilon_0}{2}\int d^3r\,|E|^2$ takes the form of the energy stored in an electric-field configuration ($\leadsto$ interpretation of ϕ as a (fictitious) electric scalar potential).

Integrate out the electron field:

$$Z = \int \mathcal{D}\overline{\psi}\mathcal{D}\psi\ e^{-S[\overline{\psi},\psi]} = \int \mathcal{D}\overline{\psi}\mathcal{D}\psi \int \mathcal{D}\phi\ e^{-S[\overline{\psi},\psi;\phi]}$$

$$= \int \mathcal{D}\phi \int \mathcal{D}\overline{\psi}\mathcal{D}\psi\ e^{-\oint d\tau \int d^3r \left(\frac{\varepsilon_0}{2}(\nabla\phi)^2 + \overline{\psi}\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right)\psi\right)}$$

$$= \int \mathcal{D}\phi\ e^{-\frac{\varepsilon_0}{2}\oint d\tau \int d^3r\,(\nabla\phi)^2}\,\mathrm{Det}\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right) = \int \mathcal{D}\phi\ e^{-S_{\text{eff}}[\phi]}$$

with

effective action $S_{\text{eff}}[\phi] = \frac{\varepsilon_0}{2}\oint d\tau \int d^3r\,(\nabla\phi)^2 - \mathrm{Tr}\ln\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right)$.

Inspection shows that this effective action has no extema away from $\phi = 0$.

To expand S_{eff} around $\phi = 0$, use the identity (if $\|A^{-1}B\| < 1$)

$$-\mathrm{Tr}\ln(A - B) = -\mathrm{Tr}\ln\left(A(1 - A^{-1}B)\right) = -\mathrm{Tr}\ln A - \mathrm{Tr}\ln(1 - A^{-1}B)$$

$$= -\ln\mathrm{Det}A + \sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Tr}(A^{-1}B)^n.$$

Auxiliary-field treatment cont'd.

In the preceding formula, set $A = \frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu \equiv G_0^{-1}$ and $B = -ie\phi$.

Then $-\operatorname{Tr}\ln\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right) = \ln \operatorname{Det} G_0 + \sum_{n=1}^{\infty} \frac{(-ie)^n}{n} \operatorname{Tr}(G_0\phi)^n$.

$n=1$: the term linear in ϕ vanishes because G_0 is constant on the diagonal and $\int d^3r\, \phi \propto \phi_{k=0}$ is absent (← overall charge neutrality; see earlier).

$n=2$:
$$\operatorname{Tr}(G_0\phi\, G_0\phi) = \frac{1}{(L^3\beta)^2} \sum_{k_1 k_2 \omega_1 \omega_2} G_0(k_1,\omega_1)\, \phi_{k_1-k_2,\omega_1-\omega_2} \times G_0(k_2,\omega_2)\, \phi_{k_2-k_1,\omega_2-\omega_1}$$
$$\equiv \frac{1}{L^3\beta} \sum_{q\omega} \Pi(q,\omega)\, \phi_{q\omega}\phi_{-q-\omega}\,,$$ where

Note $\omega = \omega_2 - \omega_1 \in \frac{2\pi}{\beta}\mathbb{Z}$

$$\Pi(q,\omega) = \frac{1}{L^3\beta} \sum_{k_1\omega_1} G_0(k_1,\omega_1)\, G_0(k_1+q,\omega_1+\omega)$$ is the polarization operator.

Terminology. Truncation of the series at quadratic order $(n=2)$ is known as the "Random Phase Approximation" (? validity: see later).

Altogether (in RPA) we have
$$S_{\text{eff}} = \frac{1}{2L^3\beta} \sum_{k\omega} \left(\varepsilon_0 |q|^2 - e^2\,\Pi(q,\omega)\right) |\phi_{q\omega}|^2 + \ldots$$

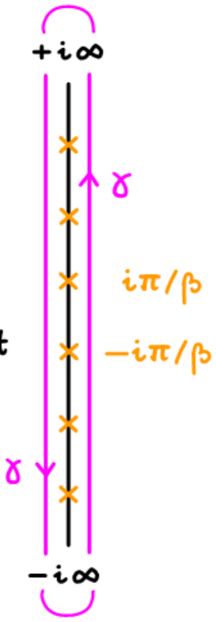
The appearance of $\Pi(q,\omega)$ suppresses fluctuations of the electric scalar potential $\phi_{q\omega}$ at long wave lengths (or small wave vector q) and small frequencies (actually, energies) ω. This is seen as follows.

We need to compute the expression

[note $G_0(k_1,\omega_1) = (-i\omega_1 + \varepsilon_{k_1} - \mu)^{-1}$]

$$\Pi(q,\omega) = \frac{1}{L^3\beta} \sum_{k_1\omega_1} \frac{1}{-i\omega_1 + \varepsilon_{k_1} - \mu}\, \frac{1}{-i(\omega_1+\omega) + \varepsilon_{k_1+q} - \mu}\,, \qquad \varepsilon_k = \frac{\hbar^2 k^2}{2m}.$$

The sum over energies ω_1 (or frequencies $\omega_1/\hbar$) is called a "Matsubara sum" (or sum over Matsubara frequencies). To perform that summation, we use the formula
$$\oint_\gamma \frac{f(z)\,dz}{e^{\beta z}+1} = \frac{2\pi i}{-\beta} \sum_{\omega_1 \in \frac{2\pi}{\beta}(\mathbb{Z} \pm 1/2)} f(i\omega_1)$$
for $f(z)$ holomorphic in a tubular neighborhood of the imaginary z-axis and with sufficient decay at infinity.



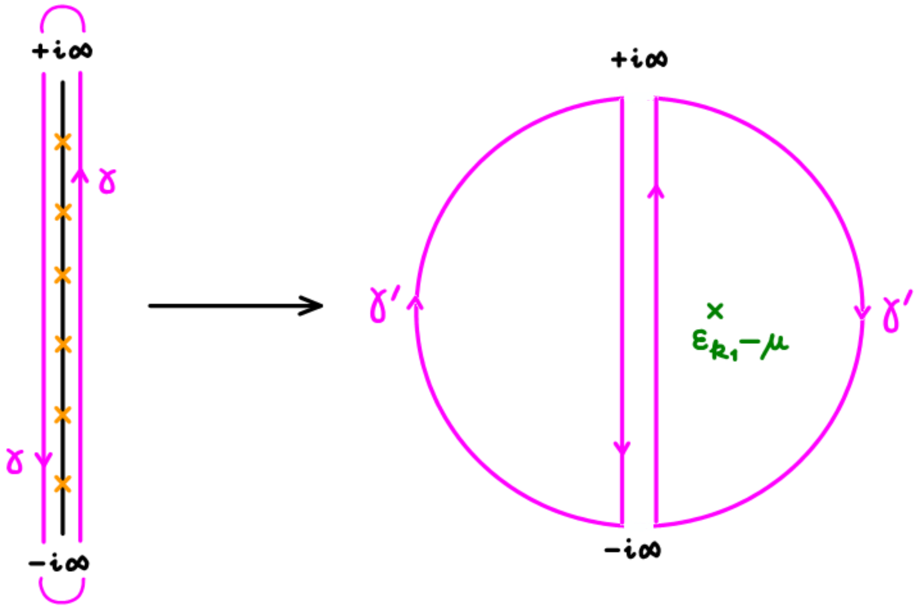
[Note $e^{\beta z}+1 = 0 \iff z \in \frac{2\pi i}{\beta}(\mathbb{Z}+1/2)$ and $\frac{d}{dz}(e^{\beta z}+1)\Big|_{\text{any zero}} = -\beta$.]

So, with $f(i\omega_1) = G_0(k_1,\omega_1)\,G_0(k_1+q,\omega_1+\omega)$ we write

$$\Pi(q,\omega) = \frac{1}{L^3\beta}\sum_{k_1}\frac{-\beta}{2\pi i}\oint_\gamma \frac{dz}{e^{\beta z}+1}\;\frac{1}{-z+\varepsilon_{k_1}-\mu}\cdot\frac{1}{-z-i\omega+\varepsilon_{k_1+q}-\mu}\;.$$

In the next step we deform the contour γ to the contour γ'.

The deformed contour γ' circulates clockwise and encloses the poles at $z=\varepsilon_{k_1}-\mu$ and $z = i\omega+\varepsilon_{k_1+k}-\mu$.



We also use $a^{-1}b^{-1} = (b-a)^{-1}(a^{-1}-b^{-1})$ with $a = -z+\varepsilon_{k_1}-\mu$ and $b = -z-i\omega+\varepsilon_{k_1+q}-\mu$. Then we obtain (writing $k_1\equiv k$)

$$\Pi(q,\omega) = \frac{1}{L^3}\sum_k \frac{1}{\varepsilon_{k+q}-i\omega-\varepsilon_k}$$

$$\cdot\,\frac{-1}{2\pi i}\oint_{\gamma'}\frac{dz}{e^{\beta z}+1}\left(\frac{1}{-z+\varepsilon_k-\mu}-\frac{1}{-z-i\omega+\varepsilon_{k+q}-\mu}\right)$$

$$= \frac{1}{L^3}\sum_k\frac{n_F(\varepsilon_{k+q})-n_F(\varepsilon_k)}{\varepsilon_{k+q}-i\omega-\varepsilon_k}\quad\text{where}\quad n_F(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

is the Fermi-Dirac distribution function. Note $n_F(\varepsilon_{k+q}-i\omega) = n_F(\varepsilon_{k+q})$

Static screening length. We now set $\omega=0$ ($\rightarrow$ static limit) and take q to be small ($\rightarrow$ limit of long wavelength). Then

$$\Pi(q,0) = \frac{1}{L^3}\sum_k\frac{n_F(\varepsilon_{k+q})-n_F(\varepsilon_k)}{\varepsilon_{k+q}-\varepsilon_k}\xrightarrow{q\text{ small}}\frac{1}{L^3}\sum_k n_F'(\varepsilon_k)$$

$$= \int \nu(\varepsilon)\,d\varepsilon\; n_F'(\varepsilon)\overset{\text{low }T}{\cong} -\nu(\varepsilon_F)$$ with $\nu(\varepsilon_F)$ the local density of states (LDOS) at the Fermi energy.

Note. In the high-density limit, the LDOS is large, thereby justifying the RPA truncation.

Effective interaction.

$$\tilde{V}_{\text{eff}}^{-1}(q) = \tilde{V}^{-1}(q) - \Pi(q,0) \cong \frac{\varepsilon_0}{e^2}|q|^2 + \nu(\varepsilon_F) \equiv \frac{\varepsilon_0}{e^2}\left(|q|^2 + \lambda^{-2}\right)$$

$$\rightsquigarrow \; V_{\text{eff}}(r-r') = \int \frac{d^3k}{(2\pi)^3}\, e^{iq\cdot(r-r')}\, \tilde{V}_{\text{eff}}(q)$$

$$= \frac{e^2}{\varepsilon_0}\int \frac{d^3}{(2\pi)^3}\, \frac{e^{iq\cdot(r-r')}}{|q|^2+\lambda^{-2}} = \frac{e^2}{4\pi\varepsilon_0}\, \frac{e^{-|r-r'|/\lambda}}{|r-r'|}\,.$$

Thus the Coulomb interaction is screened by the high-density electron gas over a length λ given by $\lambda^{-2} = \frac{e^2}{\varepsilon_0}\nu(\varepsilon_F)$.

Plasma frequency.

Consider the low-temperature limit $(\beta \longrightarrow \infty)$,

$$\Pi(q,\omega) = \frac{1}{L^3}\sum_k \frac{n_F(\varepsilon_{k+q}) - n_F(\varepsilon_k)}{\varepsilon_{k+q} - i\omega - \varepsilon_k} \xrightarrow{\beta\to\infty} \frac{1}{L^3}\left(\sum_{|k+q|<k_F} - \sum_{|k|<k_F}\right)\frac{1}{\varepsilon_{k+q}-\varepsilon_k - i\omega}$$

$$= \frac{1}{\text{vol}}\sum_{|k|<k_F}\left(\frac{1}{\varepsilon_k - \varepsilon_{k-q} - i\omega} - \frac{1}{\varepsilon_{k+q}-\varepsilon_k - i\omega}\right),$$

and specialize to the high-frequency regime (note $v_F = \frac{\hbar k_F}{m}$),

$$\Pi(q,\omega) \overset{v_F|q| \ll \omega/\hbar}{\approx} \frac{1}{\omega^2\,\text{vol}}\sum_{|k|<k_F}\left(2\varepsilon_k - \varepsilon_{k-q} - \varepsilon_{k+q}\right)$$

$$= -\frac{\hbar^2}{m}\,\frac{|q|^2}{\omega^2\,\text{vol}}\sum_{|k|<k_F} = -\frac{\hbar^2}{\omega^2}|q|^2\frac{n_0}{m}\,,$$

with n_0 the particle density $n_0 = \frac{1}{\text{vol}}\sum_{|k|<k_F}$.

Thus, $\tilde{V}_{\text{eff}}^{-1}(q) = \frac{\varepsilon_0}{e^2}|q|^2 - \Pi(q,\omega) \approx |q|^2\left(\frac{\varepsilon_0}{e^2} + \frac{\hbar^2}{\omega^2}\frac{n_0}{m}\right)$.

$\rightsquigarrow$ plasma frequency $\omega_p = \sqrt{\frac{e^2}{\varepsilon_0}\frac{n_0}{m}}$.

IV.12 Quantum Anomalies

Q: What is meant by an "anomaly"?

A: a symmetry of the classical theory which fails to carry over to the quantum theory.

First studied in the 1970-80's, anomalies have come to play a major in the contemporary physics of topological quantum matter, as a tool to classify, e.g., topological insulators and their exotic surface states.

Chiral Anomaly (D = 3+1).

Adopt the Weyl-representation for the gamma matrices.

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^\ell = \begin{pmatrix} 0 & \sigma_\ell \\ -\sigma_\ell & 0 \end{pmatrix}.$$

Introduce the chirality operator $\gamma_5 = i^{-1}\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$.

Note $\gamma_5\gamma^\mu + \gamma^\mu\gamma_5 = 0$.

Recall (from symmetries ~ conservation laws):

$$S = \int d^4x\, \bar\psi \left(\gamma^\mu \left(\tfrac{\hbar}{i}\partial_\mu - eA_\mu \right) + mc \right) \psi$$

invariant under $\psi(x) \mapsto e^{i\theta}\psi(x)$, $\bar\psi(x) \mapsto \bar\psi(x)\, e^{-i\theta}$,

$$\xrightarrow{\text{"Noether"}} \partial_\mu J^\mu = 0 \text{ for } J^\mu = e\,\bar\psi\gamma^\mu\psi \quad \text{(vector current).}$$

Now $$S\big|_{m=0} = \int d^4x\, \bar\psi \left(\gamma^\mu \left(\tfrac{\hbar}{i}\partial_\mu - eA_\mu \right) \right) \psi$$

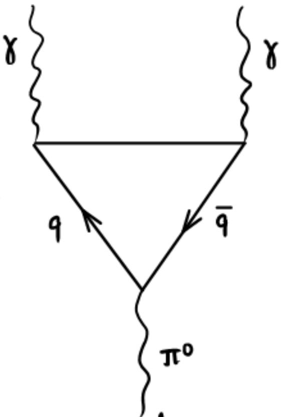
invariant under $\psi(x) \mapsto e^{i\theta\gamma_5}\psi(x)$, $\bar\psi(x) \mapsto \bar\psi(x)\, e^{+i\theta\gamma_5}$,

$$\overset{?}{\Longrightarrow} \partial_\mu J_5^\mu \overset{?}{=} 0 \text{ for } J_5^\mu = e\,\bar\psi\gamma^\mu\gamma_5\psi \quad \text{(axial current).}$$

No! The correct relation (in the quantum theory) is

$$\partial_\mu J_5^\mu = \text{const}(\hbar)\, \epsilon^{\mu\nu\lambda\rho} \underbrace{F_{\mu\nu}F_{\lambda\rho}}_{\propto E\cdot B}.$$

Example:



pion decay

Adler, Bell, Jackiw (1969; QED): axial anomaly from perturbation theory (triangle diagrams).

Fujikawa (1979): the path-integral measure is <u>not</u> invariant under axial transformations.

Chiral anomaly $(D = 1+1)$. $\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\gamma^1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

To be considered: $\mathrm{Det}\left(\gamma^\mu\left(\partial_\mu - ieA_\mu/\hbar\right)\right)$.

[Motivation / Preparation: Why consider the determinant?

For $\hat{H} = \sum_k \epsilon_k \frac{1}{2}\left(c_k^+ c_k - c_k c_k^+\right)$ consider the grand canonical partition function

$$\mathrm{Tr}\, e^{-\beta \hat{H}} = \prod_k \left(e^{\beta\epsilon_k/2} + e^{-\beta\epsilon_k/2}\right) = \mathrm{Det}\left(2\cosh(\beta H/2)\right).$$

<u>Claim</u>. $\mathrm{Tr}\, e^{-\beta\hat{H}} = \mathrm{const}\cdot \mathrm{Det}\left(\frac{\partial}{\partial t} + H\right)$ where $\frac{\partial}{\partial t}$ acts on anti-periodic functions $f : [0,\beta] \to \mathbb{C}$, $f(\beta) = -f(0)$.

<u>Verification</u> for $H \equiv h$ (a number).

$\frac{\partial}{\partial t}$ has eigenfunctions $e^{-i\omega_n t}$ with $\omega_n = \frac{2\pi}{\beta}\left(n + \frac{1}{2}\right)$ $n \in \mathbb{Z}$ Matsubara frequencies.

$$\delta \ln \mathrm{Det}\left(\frac{\partial}{\partial t} + h\right) = \delta \ln \prod_{n\in\mathbb{Z}} \left(-i\omega_n + h\right) = \sum_{n\in\mathbb{Z}} \frac{\delta h}{-i\omega_n + h} =$$

$$= \frac{1}{2}\sum_{n\in\mathbb{Z}} \frac{h\,\delta h}{\omega_n^2 + h^2} \underset{\text{Poisson summation formula}}{=} \delta h \frac{\beta}{2} \sum_{n\in\mathbb{Z}} (-1)^n e^{-\beta h |n|} = \delta \ln\left(2\cosh(\beta h/2)\right). \checkmark \;]$$

Now let $\partial_z = \frac{1}{2}(\partial_x - i\partial_y)$, $\partial_{\bar{z}} = \frac{1}{2}(\partial_x + i\partial_y)$ (imaginary time $t = iy$) and consider the Dirac operator $D = \begin{pmatrix} 0 & \partial_z + a \\ -\partial_{\bar{z}} + \bar{a} & 0 \end{pmatrix}$ where $a = -\frac{ie}{2\hbar}(A_x - iA_y)$.

Find a complex-valued function g such that $a = g^{-1}\partial_z g$. Then

$$D = \begin{pmatrix} g^{-1} & 0 \\ 0 & g^\dagger \end{pmatrix}\begin{pmatrix} 0 & \partial_z \\ -\partial_{\bar{z}} & 0 \end{pmatrix}\begin{pmatrix} g^{-1\dagger} & 0 \\ 0 & g \end{pmatrix}$$ where $g^\dagger \equiv \bar{g}$ in the present (Abelian) case.

In view of the multiplicativity of the determinant in finite dimension, one might now expect that $\mathrm{Det}\, D \overset{?}{=} \mathrm{Det}\begin{pmatrix} 0 & \partial_z \\ -\partial_{\bar{z}} & 0 \end{pmatrix}$. However, this is FALSE (unless g is unitary). The reason is that the determinant needs to be regularized, and after regularization the putative multiplicativity fails to hold.

Let $g = e^{\alpha+i\beta}$ with real-valued α, β. Then

$$D = \begin{pmatrix} e^{-\alpha-i\beta} & 0 \\ 0 & e^{\alpha-i\beta} \end{pmatrix} \begin{pmatrix} 0 & \partial_z \\ -\partial_{\bar z} & 0 \end{pmatrix} \begin{pmatrix} e^{-\alpha+i\beta} & 0 \\ 0 & e^{\alpha+i\beta} \end{pmatrix}.$$

β: parameter of a "vector" gauge transformation, which is unitary — hence not anomalous!

α: parameter of an "axial" gauge transformation.

$$D = e^{-\alpha\gamma_5} D_0 \, e^{-\alpha\gamma_5} \overset{\alpha \text{ constant}}{=} D_0 = \begin{pmatrix} 0 & \partial_z \\ -\partial_{\bar z} & 0 \end{pmatrix} \quad \text{chiral symmetry,}$$

BUT $\ln \mathrm{Det}(D) = -\frac{2}{\pi}\int d^2r \; \partial_z\alpha \; \partial_{\bar z}\alpha$ chiral anomaly.

Sketch of proof. Let $D_s = e^{-s\alpha\gamma_5} D_0 \, e^{-s\alpha\gamma_5}$, $s \in [0,1]$.

$$\mathrm{Det}(D_s) = \sqrt{\mathrm{Det}(D_s^2)}, \quad D_s^2 = \begin{pmatrix} -\Delta_s & 0 \\ 0 & -\tilde\Delta_s \end{pmatrix},$$

$$\Delta_s = e^{-s\alpha}\partial_z e^{2s\alpha}\partial_{\bar z} e^{-s\alpha}, \quad \tilde\Delta_s = e^{s\alpha}\partial_{\bar z} e^{-2s\alpha}\partial_z e^{s\alpha}.$$

Heat kernel regularization: $\displaystyle\int_\varepsilon^\infty \frac{dt}{t} e^{-th} \underset{\varepsilon \to 0+}{=} -\ln(\varepsilon h) + \overset{\text{const}}{\gamma} + \mathcal{O}(\varepsilon).$

$$\frac{d}{ds}\ln \mathrm{Det}(-\Delta_s) = \frac{d}{ds}\mathrm{Tr}\ln(-\Delta_s) \underset{\varepsilon-\text{reg}}{:=} -\frac{d}{ds}\int_\varepsilon^\infty \frac{dt}{t}\,\mathrm{Tr}\, e^{t\Delta_s}$$
$$= -\int_\varepsilon^\infty dt \; \mathrm{Tr}\, e^{t\Delta_s}\frac{d}{ds}\Delta_s .$$

Now $\displaystyle\frac{d}{ds}\Delta_s = -\alpha\Delta_s - \Delta_s\alpha + e^{-s\alpha}\partial_z 2\alpha \, e^{2s\alpha}\partial_{\bar z} e^{-s\alpha}$, so

$$\frac{d}{ds}\ln\mathrm{Det}(-\Delta_s) = 2\int_\varepsilon^\infty dt \; \mathrm{Tr}\,\alpha\left(e^{t\Delta_s}\Delta_s - e^{t\tilde\Delta_s}\tilde\Delta_s\right)$$
$$= 2\int_\varepsilon^\infty dt \frac{d}{dt}\mathrm{Tr}\,\alpha\left(e^{t\Delta_s} - e^{t\tilde\Delta_s}\right) \underset{\text{assume absence of zero modes}}{=} -2\,\mathrm{Tr}\,\alpha\left(e^{\varepsilon\Delta_s} - e^{\varepsilon\tilde\Delta_s}\right).$$

Exercise. $\displaystyle\mathrm{Tr}\,\alpha\left(e^{\varepsilon\Delta_s} - e^{\varepsilon\tilde\Delta_s}\right) \underset{\varepsilon\to 0+}{=} \frac{2s}{\pi}\int d^2r \; \partial_z\alpha \; \partial_{\bar z}\alpha .$

IV.13 Summary: Field Quantization for bosons vs. fermions

A field here is a mapping $f:$ space × time $\longrightarrow$ target space,

$$(r, t) \longmapsto f(r,t).$$

Examples: Dirac field (spinor), electromagnetic field (tensor),
Higgs field (scalar), ...

Quantization (fix a time): $f = f^{+} + f^{-}$

creates particles

choice of vacuum

annihilates particles

Invariant formulation.

0. Single-particle Hilbert space V, dual Hilbert space V^*,
Hermitian scalar product $\langle \cdot , \cdot \rangle_V$.

1. Space of fields $W = V \oplus V^*$ equipped with canonical bilinear form,

$$B: W \otimes W \longrightarrow \mathbb{C}, \quad B(v_1 + \varphi_1, v_2 + \varphi_2) = \begin{cases} \varphi_1(v_2) + \varphi_2(v_1) & \text{fermions,} \\ \varphi_1(v_2) - \varphi_2(v_1) & \text{bosons.} \end{cases}$$

2. Fock algebra (initially abstract) =
associative algebra generated by $W \oplus \mathbb{C}$ subject to the relations

$$w w' + \epsilon\, w' w = B(w, w') \cdot 1 \longleftarrow \text{unit element (central)}$$

fermions : $\epsilon = +1$, CAR, Clifford algebra $Cl(W, B)$,

bosons : $\epsilon = -1$, CCR, Weyl algebra $\mathcal{W}(W, B)$.

3. Real structure. $W \supset W_{\mathbb{R}}$ = graph of Frechet–Riesz isomorphism $V \longrightarrow V^*$,
i.e. $W_{\mathbb{R}} = \{ v + \langle v, \cdot \rangle_V \mid v \in V \}$.

Remark: $Cl(W_{\mathbb{R}}, B)$ real algebra of Majorana operators,
$\mathcal{W}(W_{\mathbb{R}}, B)$ real polynomials in position & momentum.

4. Choose a complex structure $J \in \mathrm{End}(W_{\mathbb{R}})$, $J^2 = -1_{W_{\mathbb{R}}}$, which preserves the canonical bilinear form: $\mathcal{B}(Jw, Jw') = \mathcal{B}(w, w')$.

<u>Remark</u>: a choice of complex structure determines a choice of vacuum and vice versa.

5. J- eigenspaces:

$$E_{+i}(J) \equiv \mathcal{F}^- \rightsquigarrow \text{annihilation operators: } f^-|\mathrm{vac}\rangle = 0,$$

$$E_{-i}(J) \equiv \mathcal{F}^+ \rightsquigarrow \text{creation operators: } f^+|\mathrm{vac}\rangle \neq 0.$$

<u>Note</u>: $\mathcal{B}(\mathcal{F}^-, \mathcal{F}^-) = 0 = \mathcal{B}(\mathcal{F}^+, \mathcal{F}^+)$: $\mathcal{F}^\pm$ "isotropic" (or "Lagrangian").

$$\text{Fock–Hilbert space} = \begin{cases} \Lambda(\mathcal{F}^+) & \text{fermions,} \\ S(\mathcal{F}^+) & \text{bosons,} \end{cases}$$

with Hermitian scalar product induced from $\langle \cdot , \cdot \rangle_V$.

Terminology: $\Lambda(\mathcal{F}^+) \subset Cl(W, \mathcal{B})$ exterior algebra,
$S(\mathcal{F}^+) \subset \mathcal{W}(W, \mathcal{B})$ symmetric algebra.

6. Canonical representation of Fock algebra on Fock space

fermions: $v \in \mathcal{F}^+ \longmapsto \varepsilon(v)$, $\varphi \in \mathcal{F}^- \longmapsto \iota(\varphi)$,

bosons: $v \in \mathcal{F}^+ \longmapsto \mu(v)$, $\varphi \in \mathcal{F}^- \longmapsto \delta(\varphi)$.

Example ("beyond textbook"):
canonical quantization of the free Dirac field.

1. Complex phase space $W_{\mathbb{C}} \ni \{\psi, \tilde{\psi}\}$ where spinor $\psi(x) = \begin{array}{|c|}\hline \\ \hline \\ \hline \\ \hline \\ \hline \end{array}$ solves the free Dirac equation $D\psi = 0$, $D = \gamma^\mu \partial_\mu + imc/\hbar$.

   ? Equation of motion for co-spinor $\tilde{\psi}(x) = \begin{array}{|c|c|c|c|}\hline & & & \\ \hline \end{array}$? (→ see below).

   Tautological pairing $\langle \cdot , \cdot \rangle_S$: co-spinors ⊗ spinors ⟶ functions.

2. Symmetric bilinear form $B: W_{\mathbb{C}} \otimes W_{\mathbb{C}} \longrightarrow \mathbb{C}$.

$$B(\psi^{(1)} \oplus \tilde{\psi}^{(1)}, \psi^{(2)} \oplus \tilde{\psi}^{(2)}) = B(\tilde{\psi}^{(1)}, \psi^{(2)}) + B(\tilde{\psi}^{(2)}, \psi^{(1)}),$$

$$B(\tilde{\psi}, \psi') = \int_{\Sigma_3} \langle \tilde{\psi}, \gamma^\mu \psi' \rangle_S \, \iota(\partial_\mu) \, d^4x,$$ where d^4x = space-time volume density and Σ_3 any (!) space-like 3-surface.

Note. In order for B to be independent of the (arbitrary) choice of Σ_3, we need the integrand to be closed, i.e.

$$d \, \langle \tilde{\psi}, \gamma^\mu \psi' \rangle_S \, \iota(\partial_\mu) \, d^4x = 0 .$$

This requirement will give us the equation of motion for co-spinors (if we don't know it already from another argument). Working in a Cartesian basis of Minkowski space-time we have $d \, \iota(\partial_\mu) \, d^4x = 0$, hence

$$\begin{aligned} 0 &= d \, \langle \tilde{\psi}, \gamma^\mu \psi' \rangle_S \, \iota(\partial_\mu) \, d^4x = d \langle \tilde{\psi}, \gamma^\mu \psi' \rangle_S \wedge \iota(\partial_\mu) \, d^4x \\ &= \left(\langle \tilde{\psi}, \gamma^\mu \partial_\nu \psi' \rangle_S + \langle \partial_\nu \tilde{\psi}, \gamma^\mu \psi' \rangle_S \right) \varepsilon(dx^\nu) \, \iota(\partial_\mu) \, d^4x \\ &= \left(\langle \tilde{\psi}, \gamma^\mu \partial_\mu \psi' \rangle_S + \langle \partial_\mu \tilde{\psi}, \gamma^\mu \psi' \rangle_S \right) d^4x = 0 \end{aligned}$$

$$\xRightarrow{D\psi = 0} \quad D^* \tilde{\psi} = 0, \qquad D^* = -(\gamma^\mu)^* \partial_\mu + imc/\hbar,$$

$$(\gamma^\mu)^* \tilde{\psi} := \tilde{\psi} \circ \gamma^\mu \quad \text{(pullback; canonical adjoint).}$$

3. Real structure $W_{\mathbb{C}} \supset W_{\mathbb{R}} \ni \{\psi, \bar{\psi}\}$ where $\bar{\psi} = \psi^\dagger \gamma^0$.

Recall that the spinor representation $g \mapsto S(g)$ is pseudo-unitary: $S(g)^\dagger = \gamma^0 S(g)^{-1} \gamma^0$. It follows that the real structure map $\psi \mapsto \bar{\psi}$ is Lorentz-equivariant:

$$\overline{S(g)\psi} = \psi^\dagger S(g)^\dagger \gamma^0 = \psi^\dagger \gamma^0 S(g)^{-1}$$
$$= \bar{\psi}\, S(g)^{-1} = S(g)^{-1\,*}\, \bar{\psi}.$$

Moreover, the real structure is consistent with the equations of motion:

$$D\psi = 0 \implies 0 = \overline{D\psi} = -i\frac{mc}{\hbar}\bar{\psi} + \overline{\gamma^\mu \partial_\mu \psi}$$
$$= -\Big(\underbrace{-\partial_\mu \psi^\dagger (\gamma^\mu)^\dagger \gamma^0}_{=\, \partial_\mu \bar{\psi}\, \gamma^\mu} + i\frac{mc}{\hbar}\bar{\psi}\Big) = -D^* \bar{\psi}.$$

So, postulating the real structure $\psi \mapsto \bar{\psi}$ for the space of solutions is an alternative path to getting hold of the equation of motion for co-spinors.

We could now revisit complex structure ($J \in \mathrm{End}(W_{\mathbb{R}})$, $J^2 = -1$), mode expansion, complex linear charge conjugation, CPT-theorem, ... but it's the

END of TERM

■

OUTLOOK: QFT-2 (SS 2024)

- perturbation theory: Feynman graphs (→ QED)
- spontaneous symmetry breaking: Goldstone modes
- Anderson-Higgs mechanism: theory of superconductivity
- renormalization group: ideas and practice