Quantum Field Theory – 1

(M. Zirnbauer, summer term 2020)

CHAPTER I : From Particles to Fields

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

Equations of motion (Euler-Lagrange eqn):

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

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

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

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

I.2 Stable equilibrium

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

Definition. $q^{(0)}$ is called an equilibrium (position) if $(d\mathcal{U})_{q^{(0)}} = 0$.

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

(in affine space)

$F_q = -(d\mathcal{U})_q$ is called the force in q.

(Force is a co-vector, or form, not a vector!)

$F_q(v) = -(d\mathcal{U})_q(v)$ is the (negative of the) differential change of the potential energy $\mathcal{U}$ 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

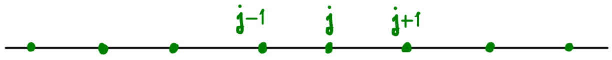
$$\mathcal{L}'(u,\dot{u}) = \frac{1}{2}\sum_{i,j}\left(A_{ij}\dot{u}_i\dot{u}_j - B_{ij}u_i u_j\right)$$

with "mass matrix" $A > 0$, and $B > 0$ for a stable equilibrium $u \equiv 0$.

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

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)

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

$u_0 \equiv u_N$ (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 ...

1.5 Continuum approximation for the harmonic chain

$$u_j(t) \to u(x,t) \, , \quad \dot{u}_j(t) \to \dot{u}(x,t) \, , \quad u_j - u_{j-1} \to a \frac{\partial}{\partial x} u(x,t) \, , \quad \sum_j \to \frac{1}{a} \int dx \; .$$

$$\mathcal{L} \to \mathcal{L}_{\text{cont}} = \frac{1}{2} \oint_0^L dx \underbrace{\left(\frac{m}{a} \dot{u}^2 - ca\, u'^2 \right)}_{\text{Lagrangian density}}$$

Derivation of equations of motion from variational principle:

Action functional : $S = \int_0^T dt \; \mathcal{L}_{\text{cont}}(u, \dot{u})$

Variation : $u(x,t) \longrightarrow u(x,t) + s\, \delta u(x,t)$

$$\delta S\Big|_u [\delta u] = \frac{d}{ds}\Big|_{s=0} \int_0^T dt \; \mathcal{L}_{\text{cont}}(u + s\delta u, \dot{u} + s\delta \dot{u})$$
$$=: \int_0^T dt \oint_0^L dx \left(\delta u(x,t) \frac{\delta \mathcal{L}}{\delta u(x,t)} + \underbrace{\delta \dot{u}(x,t) \frac{\delta \mathcal{L}}{\delta \dot{u}(x,t)}}_{\overset{\text{part.int.}}{=} - \delta u(x,t) \frac{\partial}{\partial t} \frac{\delta \mathcal{L}}{\delta \dot{u}(x,t)}} \right)$$

$$\delta S\Big|_u = 0 \Longrightarrow \frac{\delta \mathcal{L}}{\delta u(x,t)} = \frac{\partial}{\partial t} \frac{\delta \mathcal{L}}{\delta \dot{u}(x,t)} \quad \text{(Euler - Lagrange equation)}$$

Note : since our $\mathcal{L}$ depends on the displacement field only through $u' = \frac{\partial}{\partial x} u$ we have the identity $\frac{\delta \mathcal{L}}{\delta u(x,t)} = \frac{\partial}{\partial x} \frac{\delta \mathcal{L}}{\delta u'(x,t)}$.

Here $\frac{\delta \mathcal{L}}{\delta u(x,t)} = c a\, u''(x,t)$, $\frac{\delta \mathcal{L}}{\delta \dot{u}(x,t)} = \frac{m}{a}\, \dot{u}(x,t)$.

Hence $\ddot{u} = v_s^2\, u''$ (wave equation)

with $v_s = a\sqrt{\frac{c}{m}}$ (speed of sound).

Monochromatic solution of wave equation: $u(x,t) = e^{i(kx-\omega_k t)}$,

where $\omega_k = v_s |k|$.

Comparison.

	discrete	continuous
ω_k	$\Omega\,\vert 2\sin(ka/2)\vert$	$\Omega a \vert k\vert$

Observation: continuum approximation okay for small wave number ($|ka| \ll 1$)
(or large wave length $\sim 1/k$)

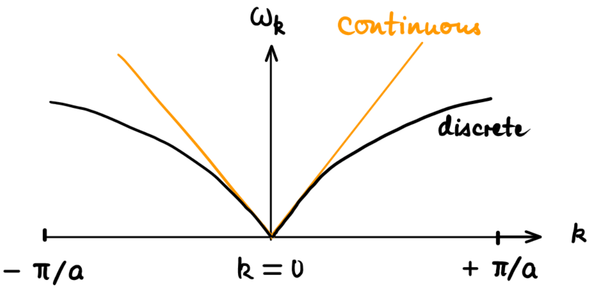
Summary: here we have an instance where the following diagram is 'commutative' for the physics at long wavelengths:

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

Lecture 02

Summary.

Harmonic chain (discrete) of particle displacements	$\mathbb{Z}_N \times \mathbb{R} \to \mathbb{R}$, $(j, t) \mapsto u_j(t)$,
is approximated, in the long wavelength limit, by a massless free scalar field (in 1+1 dimensions)	$S^1 \times \mathbb{R} \to \mathbb{R}$, $(x, t) \mapsto u(x,t)$.



I.* Tutorial on derivatives

$$\frac{\partial}{\partial x_i} x_j = \delta_{ij} .$$

i) Partial derivative is not defined until you specify the complete coordinate system!

Example (thermodynamics): $\left.\frac{\partial}{\partial p}\right|_T$ versus $\left.\frac{\partial}{\partial p}\right|_S$.

ii) Total time derivative assumes that there is some curve $t \longmapsto \gamma(t)$.

Then $\frac{d}{dt} f \equiv \frac{d}{dt}(f \circ \gamma)(t)$.

iii) Euler-Lagrange equations with Lagrangian $\mathcal{L}(q, \dot{q})$:

$$\left.\frac{\partial \mathcal{L}}{\partial q_i}\right|_{\substack{q=\gamma(t)\\ \dot{q}=\dot{\gamma}(t)}} = \frac{d}{dt} \left.\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right|_{\substack{q=\gamma(t)\\ \dot{q}=\dot{\gamma}(t)}}$$

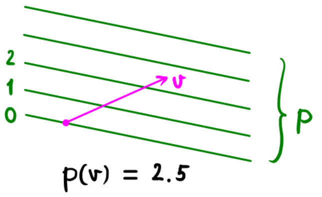
iv) What happens when $\dot{u}_j(x) \xrightarrow[\text{approx}]{\text{cont}} \frac{\partial}{\partial t} u(x,t)$?

Answer: $$\frac{\delta \mathcal{L}}{\delta u} = \frac{\partial}{\partial x} \frac{\delta \mathcal{L}}{\delta u'} + \frac{\partial}{\partial t} \frac{\delta \mathcal{L}}{\delta \dot{u}}$$

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

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



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

$$\begin{array}{rl} p: & V \longrightarrow \mathbb{R} \\ & v \longmapsto p(v) = \sum p_i v^i . \end{array}$$

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

$$\begin{array}{ccc} V & \longrightarrow & V^* , \\ v & \longmapsto & p = (d\mathcal{L})_v \end{array} .$$

In components: $p_i = f_i(v) = \dfrac{\partial \mathcal{L}}{\partial v^i}(v)$,

Inverse map: $v^i = g^i(p)$.

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

$$\mathcal{H}(p) = \sum_i p_i \, g^i(p) - \mathcal{L}(g(p)) = pv - \mathcal{L} .$$

Properties. (i) $v \longmapsto (d\mathcal{L})_v = p$ is the inverse of $p \longmapsto (d\mathcal{H})_p = v$.

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

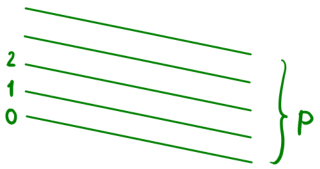
$$V \xrightarrow{\widetilde{\mathrm{Hess}}_v(\mathcal{L})} V^* \xrightarrow{\widetilde{\mathrm{Hess}}_p(\mathcal{H})} V$$

is the identity map (given that $p = (d\mathcal{L})_v$).

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

Summary.

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



I.7 Application to Harmonic Chain (continuum limit)

Recall $\mathcal{L} = \frac{1}{2} \oint_0^L dx \left(\mu \dot{u}^2 - \varkappa u'^2 \right)$; mass density μ, elastic constant $\varkappa$.

Canonical momentum: $\pi(x) = \frac{\delta \mathcal{L}}{\delta \dot{u}(x)} = \mu \dot{u}(x)$.

Hamiltonian function: $\mathcal{H} = \oint_0^L dx \left(\frac{\pi(x)^2}{2\mu} + \frac{\varkappa}{2} u'(x)^2 \right)$.

Canonical equations of motion: $\dot{u}(x) = \frac{\delta \mathcal{H}}{\delta \pi(x)} = \frac{\pi(x)}{\mu}$,

(from Hamiltonian mechanics)

$$\dot{\pi}(x) = - \frac{\delta \mathcal{H}}{\delta u(x)} = \varkappa u''(x) .$$

By eliminating $\pi(x)$ from the equations, we recover the wave equation for u:

$$\ddot{u} = \frac{\dot{\pi}}{\mu} = \frac{\varkappa}{\mu} u'' =: c^2 u'' \qquad (c = \text{speed of sound}).$$

Solutions. $u(x,t) = f_+(x-ct) + f_-(x+ct)$

The energy of a solution is constant in time:

Let, e.g., $u(x,t) = f(x-ct)$. Then

$$\pi(x,t) = \mu \dot{u}(x,t) = -\mu c\, f'(x-ct) \quad \text{and} \quad u'(x,t) = f'(x-ct).$$

$$\text{Hence} \quad \mathcal{H} = \varkappa \oint dx\, f'(x-ct)^2 = \varkappa \oint dx\, f'(x)^2 = \text{const.}$$

Info (for advanced students).

In the general setting of a field u : space(-time) $S \longrightarrow$ manifold M the vector space of generalized velocities is the tangent bundle TM pulled back by the (fixed) field map $u : S \longrightarrow M$ to a vector bundle $u^*(TM)$ over S.

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?

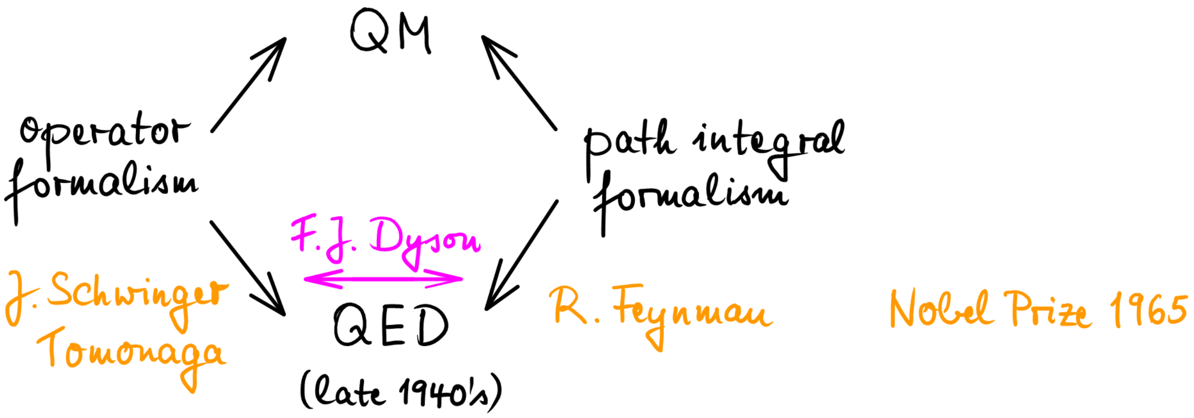
Gell-Mann: Because Feynman uses a different method than we do.

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.

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

Path integral.

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

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

Composition law:

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

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,

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

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

So $\langle x \,|\, e^{-i\Delta t H/\hbar} \,|\, y \rangle = e^{-i\Delta t\left(V(x)+V(y)\right)/2\hbar}\, \langle x \,|\, e^{-i\Delta t T/\hbar} \,|\, y \rangle + \dots$

(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:

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

In this way, Feynman arrived at the following expression for the time-T propagator:

$$\langle x' | e^{-iTH/\hbar} | x \rangle \overset{\Delta t \equiv T/N}{=} \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{N/2} \int_{x_0 \equiv x}^{x_N \equiv x'} dx_1 dx_2 \cdots dx_{N-1}$$

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

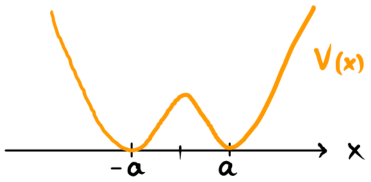
$$\overset{!!}{=:} \int_{x(0)=x}^{x(T)=x'} \mathcal{D}[x(t)] \exp\left(\frac{i}{\hbar} \int_0^T L\, dt \right) \quad \text{where} \quad L(x,\dot{x}) = \frac{m}{2} \dot{x}^2 - V(x) .$$

(functional integral over "paths" $t \mapsto x(t)$).

Note: Oscillations lead to cancellations. The approximation of stationary phase,
$0 = \delta \int_0^T L\,dt$, yields the Euler-Lagrange equation $\frac{\partial L}{\partial x} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right)$.
Its solutions are trajectories of the classical system.

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) 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):

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

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

Lecture 04.

Recap.

Quantum tunneling ↭ level splitting in a symmetric double well.

Our starting point is the formula

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

Goal. Compute the LHS from the path integral.

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

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

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

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

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.

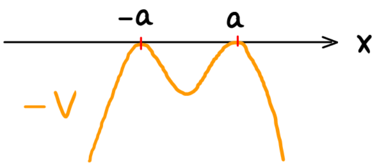
Now put $y' = a$ and $y = \mp a$ for $\begin{smallmatrix}\text{numerator}\\ \text{denominator}\end{smallmatrix}$ (see above).

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

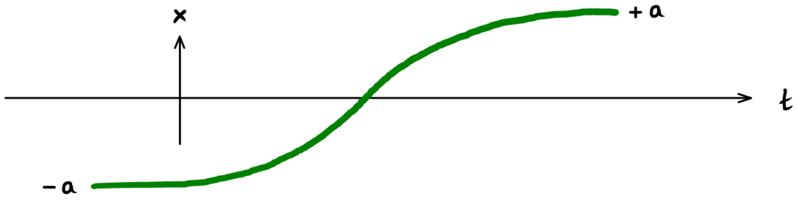
$$0 = \delta S_E \implies -m\ddot x(t) + V'(x(t)) = 0\,,$$

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 $x(t\to\mp\infty) = \mp a$, 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. $\delta S_E\big|_{x_0} = 0$:

$$S_E[x_0(t)+\delta x(t)] = S_E[x_0(t)] + 0 + \frac{1}{2}\int_0^T dt\int_0^T dt'\;\delta x(t)\,\frac{\delta^2 S_E}{\delta x(t)\,\delta x(t')}\,\delta x(t') + \dots$$

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

$$\text{and} \quad (\delta x, A\,\delta x) = \int_0^T dt\;\delta x(t)\,(A\,\delta x)(t).$$

Note $\delta x(0) = \delta x(T) = 0$.

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

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

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

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

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

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

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

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

II.4 Fluctuation Determinant

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

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

(ii) 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)

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

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

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

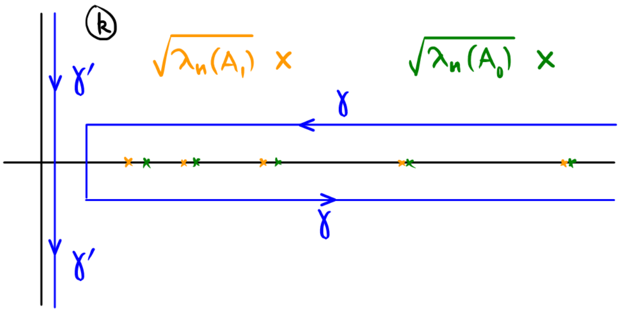
An operator A with a sequence of eigenvalues $0 < \lambda_1 < \lambda_2 < \ldots < \lambda_n < \ldots$ of quadratic growth determines a ζ-function $\zeta_A(s) = \sum_{n=1}^{\infty} \lambda_n^{-s}$ (for $\mathrm{Re}(s) > 1/2$).

Due to cancellations, the difference $\zeta_{A_1}(s) - \zeta_{A_0}(s) = \sum_{n=1}^{\infty} \left(\lambda_n(A_1)^{-s} - \lambda_n(A_0)^{-s} \right)$ 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 imaginary axis.

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 of this relation at $s = 0$ gives

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

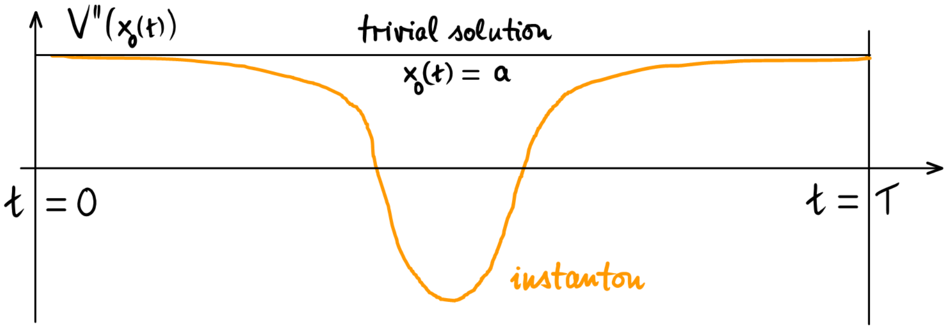
By exponentiating this relation we arrive at the desired result ∎

Remark. Thus the problem of calculating the (ratio of) functional 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

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

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

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.

From $\tanh\left(\frac{T(E_1 - E_0)}{2\hbar} \right) = \frac{\langle a | e^{-TH/\hbar} | -a \rangle}{\langle a | e^{-TH/\hbar} | a \rangle} \approx e^{-S_E^{(0)}/\hbar} \, \mathrm{Det}^{-1/2}(A_1/A_0)$

one might expect $\mathrm{Det}^{-1/2}(A_1/A_0) \sim T$. However, detailed calculations show that $\mathrm{Det}^{-1/2}(A_1/A_0)$ does <u>not</u> give the expected factor of T.

As mentioned before, the reason for the mismatch is that A_1 has a soft mode which turns into a zero mode for $T \longrightarrow \infty$. More on this in the next lecture...

Lecture 6.

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

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

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

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 <u>not</u> 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 <u>unique</u> 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.

It remains to calculate $\mathrm{Det}^{1/2}(A_0)\,\mathrm{Det}^{-1/2}(\tilde{A}_1)$. This is done below.

Result. One-instanton approximation:

$$\frac{T}{2\hbar}(E_1-E_0) = e^{-S_E^{(0)}/\hbar}\,\mathrm{Det}^{-1/2}(\tilde{A}_1/A_0)\int_0^T dt .$$

$$\text{Hence}\quad E_1-E_0 = e^{-S_E^{(0)}/\hbar}\,2\hbar\omega, \quad \omega = \mathrm{Det}^{-1/2}(\tilde{A}_1/A_0).$$

Comment. To retrieve the full power series of $\tanh((E_1-E_0)T/2\hbar)$, one needs to sum over multi-instanton configurations using the dilute instanton gas approximation (→ Exercise).

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 zero mode (if present). In the presence of a zero mode $\psi_k(1)$ vanishes as k^2 for $k^2 \longrightarrow 0$. Therefore, let $f_k \overset{\text{def}}{=} -\psi_k(1)/k^2$.

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

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

$$= \int_0^1 d\tau\,\big(u_0(\tau)A\,\psi_k(\tau) - \psi_k(\tau)A\,u_0(\tau)\big) = \int_0^1 d\tau\,\frac{d}{d\tau}\Big(-u_0(\tau)\frac{d}{d\tau}\psi_k(\tau) + \psi_k(\tau)\frac{d}{d\tau}u_0(\tau)\Big)$$

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

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

Consider now the integral $\frac{1}{2\pi i}\int_\gamma k^{-2s}\, d\ln\big((1-k^2)f_k\big)$ with the same contour γ as before. The function $k \mapsto (1-k^2)f_k$ 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: $\zeta'_{\tilde{A}}(s) = \frac{1}{2\pi i}\frac{d}{ds}\int_\gamma k^{-2s}\, d\ln\big((1-k^2)f_k\big)$.

By proceeding in the same way as before (deform the contour, etc.) one obtains the result

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

II.5 Van Vleck Formula

Use Feynman path integral in real time to construct semiclassical approximation to propagator, say for $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$.

Van Vleck formula:

$$\langle b | e^{-iTH/\hbar} | a \rangle \overset{\hbar \text{ small}}{=} \sum \sqrt{\frac{i}{2\pi\hbar} \cdot \frac{\partial^2 W_T}{\partial a \partial b}} \; e^{i W_T(a,b)/\hbar}$$

where the sum is over solutions x_{cl} of $m\ddot{x}_{cl} + V'(x_{cl}) = 0$, $x_{cl}(0) = a$, $x_{cl}(T) = b$. $W_T(a,b) = \int_0^T L(x_{cl}(t), \dot{x}_{cl}(t))\, dt$.

Warning: $\frac{\partial^2 W_T}{\partial a \partial b}$ may become zero ($\sim$ Maslov index ...).

See the Exercises for the derivation.

Remark. The Van Vleck formula leads to the Gutzwiller trace formula.

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 $a\,|0\rangle = 0$,

ground state

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

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:

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

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

Universal math allows re-interpretation:

oscillator quanta → particles (bosons).

Wavefunction 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 $v v' - v' v = 0$ (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 orthonormal basis of V. Then

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

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

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

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

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 $\mu(v) : S^n(V) \longrightarrow S^{n+1}(V) \qquad (v \in V)$

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

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

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

$\delta(\varphi) \cdot (v v') = \varphi(v) v' + \varphi(v') v$ & 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 $a_i |0\rangle = 0$, $a_i a_j^+ |0\rangle = |0\rangle \delta_{ij}$,

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

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

Proof left as an exercise.

III.* 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 $\varphi \in Y^*$).

Frechét–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,

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

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

III.3 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

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

Exercise.

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

III.4 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 $L = \sum_{ij} |i\rangle\langle i|L|j\rangle\langle j|$

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 $\sum_i \mu(Le_i)M^i{}_j = \mu\left(L\sum e_i M^i{}_j\right) = \mu\left(LMe_j\right)$

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

Lecture 09

III. 4 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 as follows. The 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. $\dim_{\mathbb{R}} W = 2$. position $q : W \longrightarrow \mathbb{R}$ momentum $p : W \longrightarrow \mathbb{R}$ $\Big\}$ local coordinates with differentials dq and dp.

$\alpha = dp \wedge dq$ (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:

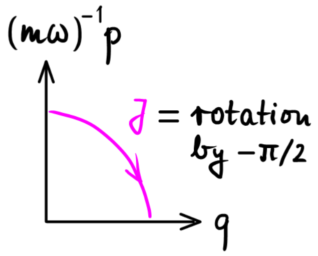
$$\alpha(w, w') = \alpha(Jw, Jw') \text{ for all } w, w' \in W.$$

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. $W = \mathrm{span}\{e_q, e_p\} \cong \mathbb{R}^2$. $Je_q = -\, m\omega\, e_p$,

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



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 $\frac{\omega}{2} g = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2$.

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

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

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

Warning (sorry): change of notation relative to the recorded video lecture

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 α restricted to $\tilde{V}$. Because α is non-degenerate it follows that $\alpha: \tilde{V} \times V \longrightarrow \mathbb{C}$ is a pairing, i.e. $\tilde{V} \longrightarrow V^*$, $\tilde{v} \longmapsto \alpha(\tilde{v}, \cdot)$ is an isomorphism.

Make this isomorphism dimensionless by scaling with Planck's constant:

$$I: \tilde{V} \longrightarrow V^*, \quad \tilde{v} \longmapsto -\frac{i}{\hbar}\alpha(\tilde{v}, \cdot).$$

Hermitian structure.

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

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

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

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

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.

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

Let $W = \mathrm{span}\left\{e_q, e_p\right\} \cong \mathbb{R}^2$,
$\alpha(e_p,e_q) = 1 = -\alpha(e_q,e_p)$, $\quad \alpha(e_p,e_p) = 0 = \alpha(e_q,e_q)$,
and $J e_q = -m\omega\, e_p$, $\ J e_p = +(m\omega)^{-1} e_q$.

✎ **Exercise:** $V = \mathbb{C}\cdot a^+$, $\quad a^+ = \frac{1}{\sqrt{2}}\left(\frac{q}{\ell} - i\frac{\ell p}{\hbar}\right)$,
$\tilde{V} \equiv V^* = \mathbb{C}\cdot a$, $\quad a = \frac{1}{\sqrt{2}}\left(\frac{q}{\ell} + i\frac{\ell p}{\hbar}\right)$.

Hint: Recall the identification $I: \tilde{V} \longrightarrow V^*$, $\ \tilde{v} \longmapsto -\frac{i}{\hbar}\alpha(\tilde{v},\cdot)$,
$V \longrightarrow \tilde{V}^*$, $\ v \longmapsto -\frac{i}{\hbar}\alpha(v,\cdot)$,
and show that $I(e_q) = \frac{i}{\hbar}p$, $\ I(e_p) = -\frac{i}{\hbar}q$.

Lecture 10.

Summary: canonical quantization for bosons.

A triple (W, α, J) (as introduced in the previous lecture) determines a "polarization"

$$W \otimes \mathbb{C} = E_{-i}(J) \oplus E_{+i}(J) \equiv V \oplus \tilde{V}$$

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

$$W^* = \tilde{V}^* \oplus V^* \cong I(V) \oplus V^* \ni I(v) + \varphi \longmapsto \mu(v) + \delta(\varphi).$$

Example: 1D harmonic oscillator.

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

Then $V^* \ni \frac{1}{\sqrt{2}} \left(\frac{q}{\ell} + i \frac{\ell p}{\hbar} \right) \equiv \varphi \longmapsto \delta(\varphi) \equiv a$

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

Unit vector $v = \frac{1}{\sqrt{2}} (e_q + iJe_q) \in V$, $\langle v, v \rangle_V = 1$.

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

III.5 Canonical quantization of 1D scalar bosonic field

Recall continuum approximation to harmonic chain (Chapter I).
⇝ scalar bosonic field in one dimension, $\varphi : [0, L] \longrightarrow \mathbb{R}$;
Dirichlet boundary conditions $\varphi(0) = \varphi(L) = 0$.

Lagrangian $\mathcal{L} = \frac{1}{2} \int_0^L dx \left(\mu \dot{\varphi}^2 - \varkappa \varphi'^2 \right)$.
Canonical momentum $\pi(x) = \mu \dot{\varphi}(x)$.
Hamiltonian function $\mathcal{H} = \frac{1}{2} \int_0^L dx \left(\frac{\pi(x)^2}{\mu} + \varkappa \varphi'(x)^2 \right)$.

Mode expansion (classical fields): $\varphi(x) = \sqrt{2/L} \sum_{n=1}^{\infty} \varphi_n \sin(\pi n x / L)$,

$$\pi(x) = \sqrt{2/L} \sum_{n=1}^{\infty} \pi_n \sin(\pi n x / L).$$

Classical Hamiltonian $\mathcal{H} = \frac{1}{2} \sum_{n=1}^{\infty} \left(\frac{\pi_n^2}{\mu} + \varkappa (n\pi/L)^2 \varphi_n^2 \right)$.

Symplectic form: $\alpha(\delta\pi, \delta\varphi) = \int_0^L dx\, \delta\pi(x)\, \delta\varphi(x)$. In terms of modes:
$\alpha(\pi_n, \varphi_{n'}) = \delta_{nn'} = -\alpha(\varphi_{n'}, \pi_n)$ and $\alpha(\pi_n, \pi_{n'}) = 0 = \alpha(\varphi_{n'}, \varphi_n)$.

Complex structure: $J \varphi_n = -\pi_n / \mu\omega_n$, $J \pi_n = +\varphi_n \mu \omega_n$,
$\omega_n = \sqrt{\frac{\varkappa}{\mu}} \cdot \frac{n\pi}{L}$ ⇝ $J(\varphi_n + i\pi_n/\mu\omega_n) = +i(\varphi_n + i\pi_n/\mu\omega_n)$.

Quantum commutator from canonical quantization: $[\varphi_n, \pi_{n'}] = i\hbar\, \delta_{nn'}$.
Expansion of modes in terms of boson creation and annihilation operators:

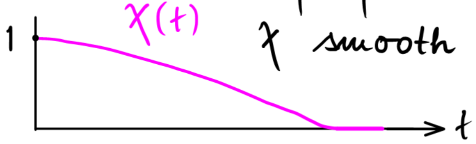
$$\varphi_n = \sqrt{\frac{\hbar}{\mu\omega_n}} (a_n + a_n^\dagger), \quad \pi_n = \sqrt{\hbar \mu \omega_n}\; i^{-1} (a_n - a_n^\dagger).$$

Quantum Hamiltonian: $\mathcal{H} = \frac{\hbar c}{2} \sum_{n=1}^{\infty} \frac{n\pi}{L} \left(a_n^\dagger a_n + a_n a_n^\dagger \right)$, $c = \sqrt{\frac{\varkappa}{\mu}}$ (speed of sound).

Zero-point energy: $E_{vac}(L) = \frac{\hbar c}{2} \sum_{n=1}^{\infty} \frac{n\pi}{L} = \infty$.

III.6 Casimir effect

Cutoff function



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

Cutoff length a.

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

$(a \to 0)$.

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,

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

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

Lecture 11.

III.7 Bogoliubov Transformations (bosons)

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

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

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"): $q_n = \frac{\ell}{\sqrt{2}}\,(a + a^+)$,

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

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

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 $\sum_{n\in\mathbb{Z}} e^{ikn} = 2\pi\,\delta(k)$, $k \in [-\pi, \pi]$. 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 $(j = 1, 2, \dots, N)$ 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: subspace spanned by the $N(2N+1)$ operators

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

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

Which Lie algebra?

Matrix representation. Consider (summation convention!)

$$\tfrac{1}{2} A^j{}_l (a_j^+ a^l + a^l a_j^+) + \tfrac{1}{2} B^{jj'} a_j^+ a_{j'}^+ - \tfrac{1}{2} C_{ll'} a^l a^{l'} \equiv \hat{X} .$$

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 $X \longmapsto \hat{X}$ is an isomorphism of Lie algebras.

Main idea of proof.

$$\hat{X} = \tfrac{1}{2} (a_j^+ \quad -a^l) \begin{pmatrix} A^j{}_{l'} & B^{jj'} \\ C_{ll'} & -A^{j'}{}_l \end{pmatrix} \begin{pmatrix} a^{l'} \\ a_{j'}^+ \end{pmatrix} \equiv \tfrac{1}{2} \gamma_\nu X^\nu{}_{\nu'} \tilde{\gamma}^{\nu'} .$$

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

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

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

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

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

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

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

More on the Exercise Sheet ...

Lecture 12.

III. 8 Fermions: 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):

$$c_i^+ c_j^+ + c_j^+ c_i^+ = 0 = c_i c_j + c_j c_i , \qquad c_i c_j^+ + c_j^+ c_i = \delta_{ij} .$$

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 ($\to$ 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),

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

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

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

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

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

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

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

What takes the role of the Weyl algebra ($\to$ bosons) in the present case of fermions?

Definition. Let V be a complex vector space. The Clifford algebra $\mathrm{Cl}(V \oplus V^*)$ 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 $\varepsilon(v) : \Lambda^n(V) \longrightarrow \Lambda^{n+1}(V) \quad (v \in V)$,

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

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

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

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

Transcription. $\varepsilon(v) \longleftrightarrow c_i^{\dagger} v^i$ 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, $L \longmapsto \varepsilon(Le_i)\,\iota(f^i) \equiv \hat{L}$, preserves commutators: $[\hat{L}, \hat{M}] = \widehat{[L,M]}$.

Hermitian conjugation. (Frechet-Riesz isomorphism γ)

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

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

Lecture 13

IV. Quantization of the Dirac Field

IV. 1 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

$$\rho = \psi^\dagger\psi, \quad \vec{j} = c\psi^\dagger\vec{\alpha}\psi.$$

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.

$\underline{\text{IV}}$.2 Hole quantization

Recall standard (particle-type) quantization:

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

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

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

Alternative (hole-type) quantization:

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

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

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

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

$$= -\,\varepsilon(f^i) \otimes \iota(He_i) = \varepsilon(-H^t f^i) \otimes \iota(e_i) = {}^{h}\widehat{H}.$$

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.

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 $\wedge(V_+ \oplus V_-^*)$, 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 ↶ 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

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

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.

Lecture 14.

Hole quantization: Dirac sea picture.

Recall $V \oplus V^* \ni v + \varphi$.

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

Cartoon. ● occupied s.p. state ○ 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"

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

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

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

H_0-stable quantization of one-body operators.

For $V = E_{>0}(H_0) \oplus E_{<0}(H_0) \equiv V_+ \oplus V_-$

and Fock space $\Lambda(V_+ \oplus V_-^*)$, recall the hybrid scheme

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

Consider some one-body operator Op of interest (e.g. local charge density):

$$\mathrm{Op} \in \mathrm{End}(V) = \begin{pmatrix} \mathrm{End}(V_+) & \mathrm{Hom}(V_-, V_+) \\ \mathrm{Hom}(V_+, V_-) & \mathrm{End}(V_-) \end{pmatrix} = \begin{pmatrix} V_+ \otimes V_+^* & V_+ \otimes V_-^* \\ V_- \otimes V_+^* & V_- \otimes V_-^* \end{pmatrix}$$

$$\curvearrowright \mathrm{Op} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} .$$

Block	**Meaning**	**Dirac notation**
$A = (Ae_i^+)\otimes f_+^i \mapsto \varepsilon(Ae_i^+)\,\iota(f_+^i)$	e^-e^- scattering	$\sum_{m,n>0} \langle m\vert A\vert n\rangle\, c_m^+ c_n$
$B = (Be_i^-)\otimes f_-^i \mapsto \varepsilon(Be_i^-)\,\varepsilon(f_-^i)$	e^-e^+ pair creation	$\sum_{m>0>n} \langle m\vert B\vert n\rangle\, c_m^+ c_n^+$
$C = (Ce_i^+)\otimes f_+^i \mapsto \iota(Ce_i^+)\,\iota(f_+^i)$	e^-e^+ pair annihln	$\sum_{m<0<n} \langle m\vert C\vert n\rangle\, c_m c_n$
$D = (De_i^-)\otimes f_-^i \mapsto :\iota(De_i^-)\,\varepsilon(f_-^i):$ $= \varepsilon(-D^t f_-^i)\,\iota(e_i^-).$	e^+e^+ scattering	$\sum_{m,n<0} \langle m\vert D\vert n\rangle \underbrace{:c_m c_n^+:}_{= -c_n^+ c_m}$

IV.3 Field quantization by mode expansion

Recall that second quantization (of say, one-body operators) proceeds in two steps:

Step (I): Convert the operator defined on the single-particle Hilbert space V into an element of the Clifford algebra $\mathrm{Cl}(V \oplus V^*)$.

Step (II): Let the Clifford algebra (and hence the given operator) act on the Fock space $\mathcal{F} = \Lambda(V)$, or $\mathcal{F} = \Lambda(V^*)$, or $\mathcal{F} = \Lambda(V_+ \oplus V_-^*)$, as the case may be.

The elements of $V \oplus V^*$ are called fields (or field operators). Owing to $\mathrm{End}(V) \cong V \otimes V^*$ the second quantization of operators is already determined by the quantization of the field.

Step (I). Denote the field (of a charged particle, and in the position representation) by $x \mapsto \Psi(x)$, $x \mapsto \Psi^+(x)$.

Clifford algebra (or canonical anticommutation) relations (CAR) for a

i. scalar fermion field: $\Psi(x)\Psi^+(x') + \Psi^+(x')\Psi(x) = \delta(x-x')$,

$$\Psi(x)\Psi(x') + \Psi(x')\Psi(x) = 0 = \Psi^+(x)\Psi^+(x') + \Psi^+(x')\Psi^+(x).$$

$H \longrightarrow \int d^3x\, \Psi^+(x)\,(H\Psi)(x)$ (H any one-body operator).

ii. Dirac spinor field: $\Psi^a(x)\Psi^+_{a'}(x') + \Psi^+_{a'}(x')\Psi^a(x) = \delta^a_{a'}\,\delta(x-x')$,

$$\Psi^a(x)\Psi^{a'}(x') + \Psi^{a'}(x')\Psi^a(x) = 0 = \Psi^+_a(x)\Psi^+_{a'}(x') + \Psi^+_{a'}(x')\Psi^+_a(x).$$

$$H \longrightarrow \int d^3x\, \Psi^+_a(x)\,(H^a{}_{a'}\Psi^{a'})(x).$$

Step ⒾⒾ.

i. Scalar fermion field, $\mathcal{F} = \Lambda(V)$, $|n\rangle$ ONB of V.

Secretly, $\Psi(x)$ corresponds to $\langle x| = \sum_n \langle x|n\rangle\langle n|$

and $\Psi^+(x)$ to $|x\rangle = \sum_n |n\rangle\langle n|x\rangle$.

Hence $\Psi(x) = \sum_n \psi_n(x)\, c_n$ and $\Psi^+(x) = \sum_n \overline{\psi_n(x)}\, c_n^+$.

$$\psi_n(x) \equiv \langle x|n\rangle$$

ii. Dirac spinor field, $\mathcal{F} = \Lambda(V_+ \oplus V_-^*)$.

$$\Psi^a(x) = \sum_{m>0} \underbrace{u_m^a(x)}_{\substack{\text{positive-energy}\\ \text{eigenspinor of } H_0}}\, c_m + \sum_{n<0} \underbrace{v_n^a(x)}_{\substack{\text{negative-energy}\\ \text{eigenspinor of } H_0}}\, c_n^+ , \quad \Psi_a^+(x) = \Psi^a(x)^\dagger .$$

Exercise. Write this out more concretely for $V = L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$.

Q: The Dirac equation can only be second-quantized as a fermionic field theory?

A: Yes, but the reason why is not so obvious ...

(cf. H. Nielsen & M. Ninomiya; ~ 10 papers, 1998 – 2015 "Dirac sea for bosons")

Bosons:

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

$$\widehat{H}_0 = {}^p\widehat{H_0}\big|_{V_+} + {}^h\widehat{H_0}\big|_{V_-} > 0 \ !$$

$$[a, a^+] = [a^+, -a]$$

Charge conjugation "mystery" resolved.

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

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

$H(0,0) \equiv H_0$. $\quad C H_0 = -H_0 C \implies C V_+ = V_-$ and $C V_- = V_+$.

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

ii. Second-quantized theory.

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

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

Lecture 15.

In the presence of an electromagnetic field the free Dirac Hamiltonian H_0 is augmented by the interaction Hamiltonian (universal)

$$H_{int} = \int d^3r \left(\phi \rho - \sum_\ell A_\ell j_\ell \right).$$

Continuity equation: $\frac{\partial}{\partial t} \rho + \mathrm{div}\, \vec{j} = 0 \;\wedge\; Q = \int d^3r\, \rho = \mathrm{const.}$

Dirac: $\rho = e\psi^\dagger\psi, \quad j_\ell = ec\psi^\dagger \alpha_\ell \psi.$

Comment / Warning.

$$\text{Charge conservation} \;\overset{\text{many texts}}{\xleftarrow{\;?\;}}\; \text{local } U(1) \text{ gauge invariance.}$$

Reasoning (?): make gauge transformation $A_\mu \longrightarrow A_\mu + \partial_\mu f$ in the action functional $S_{int} = \int d^4x\, A_\mu J^\mu$. Then

$$S_{int} \longrightarrow S_{int} + \int d^4x\, (\partial_\mu f)\, J^\mu = S_{int} - \int d^4x\, f\, \partial_\mu J^\mu .$$

Gauge invariance $\overset{?}{\Rrightarrow}$ $\partial_\mu J^\mu = 0$. NO!

Note: gauge transformations also transform the matter field, by $\psi \longrightarrow e^{ief/\hbar}\psi$, and the complete action functional is gauge-invariant: $S \longrightarrow S$.

The correct statement is that charge conservation follows from global $U(1)$ phase rotation invariance (spontaneously broken in a superconductor).

Mode expansion (schematic) of e.g. charge density:

$$\left.\begin{aligned} \psi &= u c_{ele} + v c_{pos}^\dagger \\ \psi^\dagger &= c_{ele}^\dagger u^\dagger + c_{pos} v^\dagger \end{aligned}\right\} \qquad \rho(x) = \,:e\psi^\dagger(x)\psi(x):$$

consists of 4 types of terms (cf. earlier).

Calculations in this operator form (Schwinger, Tomonaga, … > mid 1940's) are complicated! Feynman (path integral) to the rescue …

IV. 4 Feynman propagator

For later reference, supply more details on H_0-eigenspinors.

Free Dirac equation $0 = (i\hbar\partial_t - H_0)\psi$ is solved by exponential ansatz for ψ.
(or Fourier transformation)

Positive-energy solutions $\psi = u_s(k)\, e^{i(k\cdot r - \omega t)}$ with spinor $u_s(k) \in \mathbb{C}^4$ have energy eigenvalue $\hbar\omega(k) = +\sqrt{(mc^2)^2 + (\hbar k c)^2}$, have momentum $\hbar k$, $k \in (\mathbb{R}^3)^*$, and spin projection $\hbar s$ $(s = \pm 1/2)$.

Negative-energy solutions $\psi = v_s(k)\, e^{i(k\cdot r + \omega t)}$ with spinor $v_s(k) \in \mathbb{C}^4$ have energy eigenvalue $-\hbar\omega(k) = -\sqrt{(mc^2)^2 + (\hbar k c)^2}$ and momentum $\hbar k$, spin projection $\hbar s$.

Orthonormality (at fixed k):

$$u_s(k)^\dagger u_{s'}(k) = \delta_{ss'} = v_s(k)^\dagger v_{s'}(k), \quad u_s(k)^\dagger v_{s'}(k) = 0 .$$

Completeness:

$$\sum_s u_s(k) \otimes u_s(k)^\dagger = \Pi_+(k) \text{ projects on positive-energy sector (at fixed } k),$$

$$\sum_s v_s(k) \otimes v_s(k)^\dagger = \Pi_-(k) \quad \text{—"— negative —"— .}$$

Covariant form of Dirac equation. Start from

$$i\hbar \frac{\partial}{\partial t}\psi = mc^2\beta\psi + \frac{\hbar c}{i}\sum_j \alpha_j \frac{\partial}{\partial x_j}\psi .$$

Multiply from the left by $\beta / i\hbar c$. Introduce $\gamma^0 \equiv \beta$ and $\gamma^j \equiv \beta\alpha_j$.
Write $x^0 \equiv ct$. Then the Dirac equation takes its covariant form:

$$\left(\gamma^\mu \frac{\partial}{\partial x^\mu} - \frac{mc}{i\hbar}\right)\psi = 0 .$$

In the presence of an electromagnetic field, replace $\frac{\partial}{\partial x^\mu} \longrightarrow \frac{\partial}{\partial x^\mu} - \frac{ie}{\hbar}A_\mu$.

The gamma matrices satisfy $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = -2Q^{\mu\nu}$ (Minkowski metric tensor with signature $(-,+,+,+)$) and thus are the generators of a Clifford algebra $Cl(\mathbb{R}^4, Q)$.

Transformation law for spinors. Consider the Lorentz group $SO(1,3)$.

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

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

Here $g \longmapsto S(g)$ 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 $\mathrm{Lie}\, SO(1,3)$).
2. Convert the linear transformation $X : \mathbb{R}^4 \longrightarrow \mathbb{R}^4$ into a skew-symmetric bilinear form $\tilde{X} : \mathbb{R}^4 \times \mathbb{R}^4 \longrightarrow \mathbb{R}$ 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 $S(e^X) = \exp\left(-\frac{1}{8} \tilde{X}_{\mu\nu} [\gamma^\mu, \gamma^\nu]\right)$.

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

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

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

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

Info. The spinor representation $g \longmapsto S(g)$ 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 $\mathrm{Spin}(1,3)$, a 2:1 cover of $SO(1,3)$.

$$\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0$$

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

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

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

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.

Remark. One can arrange for $U_s(k) \propto u_s(k)$ and $V_s(k) \propto v_s(k)$ but the normalization is different:

$$U_s(k)^\dagger \gamma^0 U_{s'}(k) = U_s(0)^\dagger S(g)^\dagger \gamma^0 U_{s'}(k) = U_s(0)^\dagger \gamma^0 S(g)^{-1} U_{s'}(k) = U_s(0)^\dagger \gamma^0 U_{s'}(0) = \delta_{ss'}.$$

Similarly, $V_s(k)^\dagger \gamma^0 V_{s'}(k) = V_s(0)^\dagger \gamma^0 V_{s'}(0) = -\delta_{ss'}$.

QFT convention $\overline{U} \equiv U^\dagger \gamma^0$ (not the complex conjugate, very sorry!)

Completeness: $\sum_s \left(U_s(k)\overline{U}_s(k) - V_s(k)\overline{V}_s(k) \right) = 1_{4\times 4}$.

Exercise. $U_s(k)^\dagger U_{s'}(k) = \delta_{ss'} \frac{\hbar\omega(k)}{mc^2} = V_s(k)^\dagger V_{s'}(k)$.

Mode expansion revisited.

$k_\mu x^\mu \equiv k\cdot r - \omega(k) t, \quad \omega(k) > 0$

$$\psi(x) = \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{mc^2}{\hbar\omega(k)}} \sum_s \left(e^{ik_\mu x^\mu} U_s(k)\, c_{+,s}(k) + e^{-ik_\mu x^\mu} V_{-s}(-k)\, c^+_{-,s}(k) \right).$$

Comment. $V_-^* \ni \langle k| \longmapsto \varepsilon(\langle k|) \equiv c_-^+(-k)$.

Lecture 16.

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

$$\psi^a(x) = \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{mc^2}{\hbar\omega(k)}} \sum_s \left(e^{ik_\mu x^\mu} U_s(k)^a\, c_{+,s}(k) + e^{-ik_\mu x^\mu} V_{-s}(-k)^a\, c^+_{-,s}(k) \right),$$

$$\bar\psi_b(y) = \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{mc^2}{\hbar\omega(k)}} \sum_s \left(e^{-ik_\mu y^\mu} c^+_{+,s}(k)\, \bar U_s(k)_b + e^{ik_\mu y^\mu} c_{-,s}(k)\, \bar V_{-s}(-k)_b \right).$$

$$\Longrightarrow G^a{}_b(x,y) = \begin{cases} + \displaystyle\int \frac{d^3k}{(2\pi)^3} \frac{mc^2}{\hbar\omega(k)}\, e^{ik_\mu(x^\mu - y^\mu)} \sum_s U_s(k)^a\, \bar U_s(k)_b \ , \\ - \displaystyle\int \frac{d^3k}{(2\pi)^3} \frac{mc^2}{\hbar\omega(k)}\, e^{-ik_\mu(x^\mu - y^\mu)} \sum_s V_s(-k)^a\, \bar V_s(-k)_b \ . \end{cases}$$

Exercise.

$$\sum_s U_s(k)^a\, \bar U_s(k)_b = \tfrac{1}{2}\left(1 - \gamma^\mu \frac{\hbar k_\mu}{mc}\right)^a{}_b ,$$

$$\sum_s V_s(k)^a\, \bar V_s(k)_b = -\tfrac{1}{2}\left(1 + \gamma^\mu \frac{\hbar k_\mu}{mc}\right)^a{}_b .$$

On the notion of propagator: free Schrödinger particle (non-relativistic).

Heaviside function $\theta(t) = \begin{cases} 1 & t>0 , \\ 0 & t<0 . \end{cases}$

$$G(r,t;r',0) \equiv \langle r |\, e^{-itH_0/\hbar} \,| r' \rangle\, \theta(t)$$

$$= \sqrt{\frac{m}{2\pi i\hbar t}}^{\,3} e^{+im\frac{(r-r')^2}{2t\hbar}}\,\theta(t) = \int \frac{d^3k}{(2\pi)^3}\, e^{ik\cdot(r-r') - i\frac{\hbar k^2}{2m}t}\,\theta(t) .$$

Now $e^{-i\frac{\hbar k^2}{2m}t}\,\theta(t) = i \displaystyle\int_{\mathbb{R}} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega + i\varepsilon - \hbar k^2/2m}$.

Hence $G(r,t;r',t') = i \displaystyle\int_{\mathbb{R}^4} \frac{d^3k\, d\omega}{(2\pi)^4} \frac{e^{ik\cdot(r-r') - i\omega(t-t')}}{\omega + i\varepsilon - \hbar k^2/2m}$.

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 $\tilde{G} = G$.

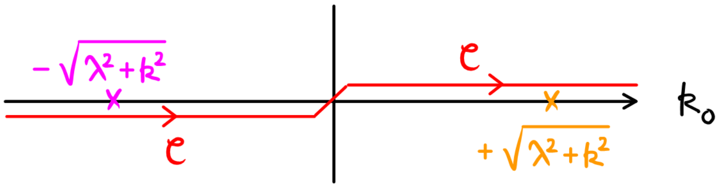
$$D^{-1} = \left(\not{\partial} - \frac{mc}{i\hbar}\right)^{-1} = \left(\not{\partial} - \frac{mc}{i\hbar}\right)^{-1}\left(\not{\partial} + \frac{mc}{i\hbar}\right)^{-1}\left(\not{\partial} + \frac{mc}{i\hbar}\right) = \left(\not{\partial}^2 + (mc/\hbar)^2\right)^{-1}\left(\not{\partial} + \frac{mc}{i\hbar}\right),$$

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

$$(D^{-1})^a{}_b(x,y) = \begin{cases} \displaystyle\int \frac{d^3k}{(2\pi)^3} \frac{mc^2}{\hbar\omega(k)}\, e^{ik_\mu (x-y)^\mu}\, \frac{1}{2}\left(1 - \gamma^\mu \frac{\hbar k_\mu}{mc}\right)^a{}_b & \text{if } x^0 > y^0, \\ \text{same with } k_0 = -\omega(k)/c \longrightarrow k_0 = +\omega(k)/c & \text{if } x^0 < y^0. \end{cases}$$

Conclusion: $(D^{-1})^a{}_b(x,y) = G^a{}_b(x,y) = \langle \text{vac} | T(\psi^a(x)\, \bar{\psi}_b(y)) | \text{vac} \rangle$
for the choice $\mathcal{C}$ of energy integration contour.

Stückelberg (1941): interpretation of positron as negative-energy electron traveling backward in time. Feynman (1947).

Lecture 17.

IV. 5 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.

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^\ell = \begin{pmatrix} 0 & \sigma_\ell \\ -\sigma_\ell & 0 \end{pmatrix}.$$

In the limit of massless particles the Dirac equation for $\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}$ splits into two equations:

$$(\partial_0 - ieA_0/\hbar)\psi_R + \sum_\ell \sigma_\ell(\partial_\ell - ieA_\ell/\hbar)\psi_R = 0,$$

$$(\partial_0 - ieA_0/\hbar)\psi_L - \sum_\ell \sigma_\ell(\partial_\ell - ieA_\ell/\hbar)\psi_L = 0.$$

Concise notation.

Introduce $\gamma_5 = i^{-1}\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$ (chirality operator),

$$\psi_L = \tfrac{1}{2}(1+\gamma_5)\psi = +\gamma_5\psi_L, \quad \psi_R = \tfrac{1}{2}(1-\gamma_5)\psi = -\gamma_5\psi_R.$$

Note $\gamma_5\gamma^\mu + \gamma^\mu\gamma_5 = 0.$

Recall $\partial_\mu J^\mu = 0$ for $J^\mu = e\bar{\psi}\gamma^\mu\psi$ (vector current).

Based on the symmetry (of the classical field theory)

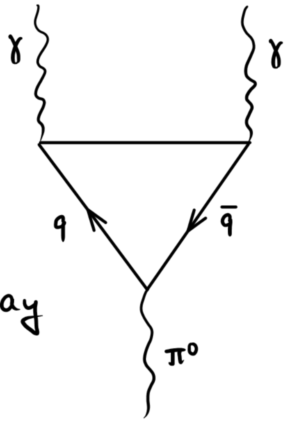
$$\gamma^\mu(\partial_\mu - ieA_\mu/\hbar) \equiv D = e^{i\alpha\gamma_5} D \, e^{i\alpha\gamma_5} \quad (\alpha = \text{const})$$

one also expects $\partial_\mu J_5^\mu = 0$ for $J_5^\mu = e\bar{\psi}\gamma_5\gamma^\mu\psi$ (axial current).

However, the correct result (for the quantum theory) is

$$\partial_\mu J_5^\mu = \text{const}(\hbar) \; \epsilon^{\mu\nu\lambda\rho} \underbrace{F_{\mu\nu}F_{\lambda\rho}}_{\propto \, E\cdot B}.$$

Adler, Bell, Jackiw (1969; QED): axial anomaly from perturbation theory (triangle diagrams). Example: pion decay



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.

For $\hat{H} = \sum_k \epsilon_k \frac{1}{2}(c_k^+ c_k - c_k c_k^+)$ consider the grand canonical partition function

$$\mathrm{Tr}\, e^{-\beta \hat{H}} = \prod_k \left(e^{\beta\epsilon_k/2} + e^{-\beta\epsilon_k/2}\right) = \det\left(2\cosh(\beta H/2)\right).$$

Claim. $\mathrm{Tr}\, e^{-\beta\hat{H}} = \mathrm{const}\cdot \mathrm{Det}\left(\frac{\partial}{\partial t} + H\right)$ where $\frac{\partial}{\partial t}$ acts on anti-periodic functions $f : [0,\beta] \to \mathbb{C}$, $f(\beta) = -f(0)$.

Verification for $H \equiv h$ (a number).

$\frac{\partial}{\partial t}$ has eigenfunctions $e^{-i\omega_n t}$ with $\omega_n = \frac{2\pi}{\beta}(n + \frac{1}{2})$ $\quad n \in \mathbb{Z}$ Matsubara frequencies.

$$\delta \ln \mathrm{Det}\left(\frac{\partial}{\partial t} + h\right) = \delta \ln \prod_{n\in\mathbb{Z}} (-i\omega_n + h) = \sum_{n\in\mathbb{Z}} \frac{\delta h}{-i\omega_n + h} =$$

$$= \frac{1}{2}\sum_{n\in\mathbb{Z}} \frac{h\,\delta h}{\omega_n^2 + h^2} \underset{\text{Poisson summation formula}}{=} \delta h\, \frac{\beta}{2} \sum_{n\in\mathbb{Z}} (-1)^n e^{-\beta h|n|} = \delta \ln\left(2\cosh(\beta h/2)\right). \checkmark$$

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 $\ln \mathrm{Det}(D) = -\frac{2}{\pi} \int d^2 r \, \partial_z \alpha \, \partial_{\bar z} \alpha$ 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: $\displaystyle\int_\varepsilon^\infty \frac{dt}{t} e^{-th} \underset{\varepsilon \to 0+}{=} -\ln(\varepsilon h) + \overset{\text{const}}{\gamma} + O(\varepsilon).$

$$\frac{d}{ds} \ln \mathrm{Det}(-\Delta_s) = \frac{d}{ds} \mathrm{Tr} \ln(-\Delta_s) \underset{\varepsilon-\text{reg}}{:=} -\frac{d}{ds} \int_\varepsilon^\infty \frac{dt}{t} \mathrm{Tr}\, e^{t\Delta_s}$$

$$= -\int_\varepsilon^\infty dt \, \mathrm{Tr}\, e^{t\Delta_s} \frac{d}{ds} \Delta_s .$$

Now $\frac{d}{ds} \Delta_s = -\alpha\Delta_s - \Delta_s \alpha + e^{-s\alpha} \partial_z 2\alpha \, e^{2s\alpha} \partial_{\bar z} e^{-s\alpha}$, 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. $\mathrm{Tr}\, \alpha \left(e^{\varepsilon\Delta_s} - e^{\varepsilon\tilde\Delta_s} \right) \underset{\varepsilon \to 0+}{=} \frac{2s}{\pi} \int d^2 r \, \partial_z \alpha \, \partial_{\bar z} \alpha .$

Lecture 18.

V. Fermionic Path Integral

V.1 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 $d\xi \equiv \frac{\partial}{\partial \xi}$ (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 $\int_F : \Lambda(V^*) \longrightarrow \mathbb{C}$.

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

Demand $\int \iota(v) \psi = 0$ ($\curvearrowleft$ "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:

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

Definition (Grassmann integral): $\int_\xi f := f^{(N)}_{12\dots N} = \dfrac{\partial^N}{\partial\xi^N\dots\partial\xi^2\partial\xi^1} f$.

Remark. Grassmann integration is nothing but differentiation!

V.2 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: $\prod_{\mu=1}^{N} \dfrac{\partial^2}{\partial\xi^\mu\partial\bar\xi_\mu}$.

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

CLAIM. $\int_\xi \exp\left(\sum_{\mu\nu} A^\mu_\nu\, \bar\zeta_\mu \zeta^\nu\right) = \mathrm{Det}(A).$

Proof.
$$\int_\xi \exp\left(\sum_{\mu\nu} A^\mu_\nu\, \bar\zeta_\mu \zeta^\nu\right) = \frac{1}{N!} \int_\xi \left(\sum_{\mu\nu} A^\mu_\nu\, \bar\zeta_\mu \zeta^\nu\right)^N$$
$$= \frac{1}{N!} \int_\xi \sum_{\pi,\pi'\in S_N} A^{\pi(1)}_{\pi'(1)}\, \bar\zeta_{\pi(1)} \zeta^{\pi'(1)} \dots A^{\pi(N)}_{\pi'(N)}\, \bar\zeta_{\pi(N)} \zeta^{\pi'(N)} .$$
$$= \frac{1}{N!} \sum_{\pi,\pi'\in S_N} \mathrm{sgn}(\pi)\,\mathrm{sgn}(\pi')\, A^{\pi(1)}_{\pi'(1)} \cdots A^{\pi(N)}_{\pi'(N)} = \sum_{\pi\in S_N} \mathrm{sgn}(\pi)\, A^{\pi(1)}_1 \dots A^{\pi(N)}_N = \mathrm{Det}(A)$$

"Real" Gaussian Berezin integral — Pfaffian.

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 $e_1, \dots, e_N$ $(e^\mu \equiv \xi^\mu)$:

$$f \in \Lambda(W^*) \mapsto \int_\xi f := \frac{\partial^N}{\partial\xi^N \dots \partial\xi^2 \partial\xi^1} f .$$

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

Examples. N odd $\rightsquigarrow \mathrm{Pf}(A) \equiv 0$. $\quad N = 2$: $\mathrm{Pf}(A) = A_{12}$.

$N = 4$: $\mathrm{Pf}(A) = A_{12} A_{34} - A_{13} A_{24} + A_{14} A_{23}$.

V.3 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 $\mathrm{Cl}(W)$ with generators c_i^+, c_i.

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

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

Convention: 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

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

Remark. 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 anticommutator 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):

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

Lecture 19.

Conceptual proof.

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

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

[Info: "Irreducible" means that there exists no subspace $\mathcal{U} \subset \wedge(V)$ which is invariant $\left(Cl(V \oplus V^*)\, \mathcal{U} \subset \mathcal{U} \right)$ 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 $\Pi_0 T_\zeta^{-1} c_i^+ = \Pi_0 \left(T_\zeta^{-1} c_i^+ T_\zeta \right) T_\zeta^{-1}$.

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

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

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

Derivation of functional integral.

$$\mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr}\left(Id_{\Lambda V}\, e^{-\frac{1}{2}\beta H}\, Id_{\Lambda V}\, e^{-\frac{1}{2}\beta H} \right)$$

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

Warning:

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

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

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

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

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

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

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

Continue the derivation of the functional integral:

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

The essential building block is $\Pi_0 T_\xi^{-1}\, e^{-\frac{1}{2}\beta\hat{H}}\, T_{\xi'} \Pi_0$.

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

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

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

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

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

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

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

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

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

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

$$\mathrm{Tr}\, e^{-\beta\hat{H}} = \lim_{M\to\infty} \int d^N\bar{\xi}_1\, d^N\xi_1 \cdots \int d^N\bar{\xi}_M\, d^N\xi_M$$

$$\exp \sum_{k=2}^{M} \left(\bar{\xi}_k \xi_{k-1} - \tfrac{1}{2}\bar{\xi}_k \xi_k - \tfrac{1}{2}\bar{\xi}_{k-1}\xi_{k-1} - \tfrac{\beta}{M}\mathcal{H}(\bar{\xi}_k, \xi_{k-1}) \right)$$

$$\exp \left(\bar{\xi}_1(-\xi_M) - \tfrac{1}{2}\bar{\xi}_1\xi_1 - \tfrac{1}{2}\bar{\xi}_M\xi_M - \tfrac{\beta}{M}\mathcal{H}(\bar{\xi}_1, -\xi_M) \right).$$

Assuming the continuum limit (justification?!) and changing notation $\xi \to \psi$ one writes the result in the form

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

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

Lecture 20.

Recap: fermionic path integral for partition function (imaginary time β):

$$\mathrm{Tr}\, e^{-\beta\widehat{H}} = \int \mathcal{D}\bar\psi\, \mathcal{D}\psi \;\exp - \oint_0^\beta d\tau \left(\bar\psi\, \partial_\tau \psi + \mathcal{H}(\bar\psi, \psi)\right)$$

infinitely many derivatives ($\rightsquigarrow$ need to establish computational rules).
$\mathcal{H}(\bar\psi,\psi)$ from normal-ordered Hamiltonian $\widehat{H} = \mathcal{H}(c^+, c)$ by the substitution $c \longrightarrow \psi$, $c^+ \longrightarrow \bar\psi$. Antiperiodic boundary conditions $\psi(\beta) = -\psi(0)$, $\bar\psi(\beta) = -\bar\psi(0)$.

Remark: encompasses both free fermions and interacting systems.

TEST. $V = \mathbb{C}$, $\widehat{H} = h\, c^+ c$ (single mode, $h>0$),

$$\mathrm{Tr}\, e^{-\beta\widehat{H}} = 1 + e^{-\beta h}.$$

$$\text{Path integral} = \int \mathcal{D}\bar\psi\, \mathcal{D}\psi \; e^{-\oint_0^\beta d\tau\, \bar\psi(\partial_\tau + h)\psi} = \mathrm{Det}(\partial_\tau + h)$$

needs regularization, by the precise definition of $\int \mathcal{D}\bar\psi\,\mathcal{D}\psi$

$$\delta \ln \mathrm{Det}(\partial_\tau + h) = \delta\, \mathrm{Tr} \ln(\partial_\tau + h) = \mathrm{Tr}\,(\partial_\tau + h)^{-1}\, \delta h = \ldots$$

Antiperiodic b.c. $\rightsquigarrow$ $e^{-i\omega_m \tau}\Big|_{\tau=\beta} = -1 \implies \omega_m = \frac{2\pi}{\beta} m, \quad m \in \mathbb{Z} + \frac{1}{2}$.

$$\ldots = \delta h \sum_{m \in \mathbb{Z}+\frac{1}{2}} (-i\omega_m + h)^{-1}$$

DIVERGENT SUM ($\rightsquigarrow$ time-continuum limit; needs cutoff).

$$= \frac{\beta\,\delta h}{2\pi} \int_{\mathbb{R}} \frac{d\omega}{-i\omega + h} \sum_{n\in\mathbb{Z}} (-1)^n e^{-i\beta\omega n} = \frac{\beta\,\delta h}{2\pi} \sum_{n \in \mathbb{Z}} (-1)^n \int_{\mathbb{R}} d\omega\, \frac{e^{-i\beta\omega n}}{-i\omega + h}$$

$$= \beta\,\delta h \sum_{n \geq 1} (-1)^n e^{-\beta h n} = \beta\,\delta h\, \frac{-e^{-\beta h}}{1 + e^{-\beta h}} = \delta \ln\left(1 + e^{-\beta h}\right). \;✓$$

Remark on antiperiodic boundary conditions.

Koszul sign rule ($c^+\zeta = -\zeta c^+$ etc.) fits perfectly with the supertrace:

$$\mathrm{STr}_{\wedge(V)} = + \mathrm{Tr}_{\wedge^{\text{even}}(V)} - \mathrm{Tr}_{\wedge^{\text{odd}}(V)} .$$

$$V = \mathbb{C} : \quad \mathrm{Tr}\,(c c^+) = 1 = \mathrm{Tr}\,(c^+ c)$$

BUT $\quad \mathrm{STr}\,(c c^+) = 1 = - \mathrm{STr}\,(c^+ c)$.

Hence $\mathrm{STr}\, e^{-\beta \widehat{H}}$ = same path integral with periodic boundary conditions.

Real-time path integral:

$$\mathrm{Tr}\, e^{-iT\widehat{H}/\hbar} = \int \mathcal{D}\bar{\psi}\, \mathcal{D}\psi \;\; \exp - \oint_0^T dt \left(\bar{\psi}\, \partial_t \psi + \tfrac{i}{\hbar}\, \mathcal{H}(\bar{\psi}, \psi) \right)$$

and antiperiodic $\bar{\psi}, \psi$.

Another remark. The path-integral method applies in particular to the second-quantized Dirac theory (in fact, that's where it celebrated its first major successes by the pioneering work of Feynman).

$$\widehat{H}_{\text{Dirac}} \equiv \mathcal{H}(c^+, c) \xrightarrow{\text{P.I.}} \mathcal{H}(\zeta^+, \zeta)$$

creates e^-, e^+ $\nearrow$ $\qquad$ $\nwarrow$ annihilates

Manipulate the positron (e^+) sector (schematic): $\zeta^+_{e^+} \zeta_{e^+} \equiv \psi_{e^+} \psi^+_{e^+} = - \psi^+_{e^+} \psi_{e^+}$.

$\leadsto$ Real-time path integral action $= \int dt \int d^3r \left(\psi^+ \partial_t \psi + \frac{i}{\hbar} \psi^+ H \psi \right)$

$= \int d^4x\; \bar{\psi} \left(\gamma^\mu \partial_\mu + i \frac{mc}{\hbar} \right) \psi$ where $\bar{\psi} = \psi^+ \gamma^0$. $\qquad$ first quantized Dirac Hamiltonian

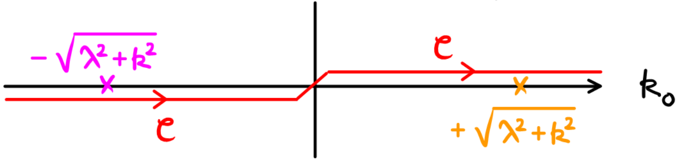
Minimal coupling $\partial_\mu \longrightarrow \partial_\mu - i \frac{e}{\hbar} A_\mu$.

More on the path integral for the Dirac theory.

Recall the time-ordered one-particle Green's function:

$$\langle vac|\mathcal{T}(\Psi^a(x)\bar\Psi_b(y))|vac\rangle = G^a{}_b(x,y) \overset{!}{=} (D^{-1})^a{}_b(x,y), \quad D = \gamma^\mu\partial_\mu + imc/\hbar .$$

Feynman propagator D^{-1}



So far (!) just an observation. Accident? No! Follows directly from fermionic path integral:

$$G^a{}_b(x,y) = \lim_{\varepsilon\to 0+} \lim_{T\to\infty\cdot e^{-i\varepsilon}} \frac{\mathrm{Tr}\, e^{-i\hat H T/2\hbar}\, \mathcal{T}(\Psi^a(x)\bar\Psi_b(y))\, e^{-i\hat H T/2\hbar}}{\mathrm{Tr}\, e^{-i\hat H T/\hbar}} .$$

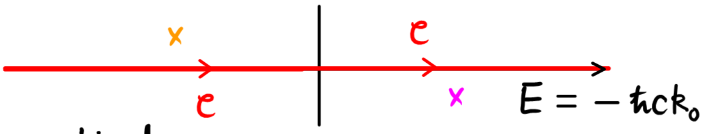
Since T occurs in the combination $\hat H T$, the factor $e^{-i\varepsilon}$ in T can be transferred to $\hat H$, thereby moving the eigenvalues of $\hat H$ (which are all positive but for the ground-state energy) into the lower half of the complex energy plane.

Use formulas 1. and 2. (from Lecture 19) 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

$$G^a{}_b(x,y) = \lim_{T\to\infty} \frac{1}{Z_1}\int \mathcal{D}\bar\psi\, \mathcal{D}\psi\; e^{iS/\hbar}\, \psi^a(x)\bar\psi_b(y), \quad S = \int d^4x\, \bar\psi\left(\gamma^\mu\partial_\mu + i\tfrac{mc}{\hbar}\right)\psi .$$

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 (~ 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.

Lecture 21

V.4 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

$$\langle \text{local density} \rangle = \frac{1}{Z}\,\mathrm{Tr}\left(c^\dagger(x)\, c(x)\; e^{-\beta(H-\mu n)}\right),$$

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 $S = \sum_{i,j} \bar\zeta_i A_{ij} \zeta_j$.

Def (for $\mathrm{Det}\, A \neq 0$):

$$\langle f(\zeta,\bar\zeta)\rangle \overset{\text{def}}{=} \frac{\int d^N\bar\zeta\, d^N\zeta\; f(\zeta,\bar\zeta)\; e^{-\sum_{i,j}\bar\zeta_i A_{ij}\zeta_j}}{\int d^N\bar\zeta\, d^N\zeta\; e^{-\sum_{i,j}\bar\zeta_i A_{ij}\zeta_j}}.$$

Sign convention: $\int d\bar\zeta\, d\zeta\; e^{-\bar\zeta a \zeta} \equiv \frac{\partial^2}{\partial\bar\zeta\,\partial\zeta}\left(1 - a\,\bar\zeta\zeta\right) = a\,\frac{\partial}{\partial\bar\zeta}\,\frac{\partial}{\partial\zeta}\,\zeta\bar\zeta = a.$

⇝ Generalization $\int (d\bar\zeta\, d\zeta)^N\, e^{-\sum_{i,j}\bar\zeta_i A_{ij}\zeta_j} = \mathrm{Det}(A).$

Fact (Wick's Theorem for complex fermions):

$$\langle \zeta_{j_1}\bar\zeta_{i_1}\,\zeta_{j_2}\bar\zeta_{i_2}\cdots\zeta_{j_n}\bar\zeta_{i_n}\rangle = \sum_{\pi\in S_n}\mathrm{sgn}(\pi)\,\langle\zeta_{j_1}\bar\zeta_{i_{\pi(1)}}\rangle\,\langle\zeta_{j_2}\bar\zeta_{i_{\pi(2)}}\rangle\cdots\langle\zeta_{j_n}\bar\zeta_{i_{\pi(n)}}\rangle.$$

Sketch of proof. Consider the generating functional (with Grassmann variables $\eta, \bar\eta$ as "sources") $Z[\eta,\bar\eta] := \int (d\bar\zeta\, d\zeta)^N\, e^{-\sum_{i,j}\bar\zeta_i A_{ij}\zeta_j + \sum_i \bar\zeta_i\eta_i + \sum_j \bar\eta_j\zeta_j}$

$$= \int (d\bar\zeta\, d\zeta)^N\, e^{-\sum_{i,j}(\bar\zeta - \bar\eta A^{-1})_i A_{ij} (\zeta - A^{-1}\eta)_j}\; e^{+\sum_{ij}\bar\eta_i A^{-1}_{ij}\eta_j}.$$

Now use the substitution rule (Berezin) with $\zeta' = \zeta - A^{-1}\eta$, $\bar\zeta' = \bar\zeta - \bar\eta A^{-1}$ and $\int (d\bar\zeta\, d\zeta)^N = \int (d\bar\zeta' d\zeta')^N$ to obtain $Z[\eta,\bar\eta]/Z[0,0] = e^{\sum_{ij}\bar\eta_i A^{-1}_{ij}\eta_j}$.

The desired result then follows by taking multiple derivatives with respect to $\eta,\bar\eta$ at zero:

$$\langle \zeta_j\bar\zeta_i\rangle = \left.\frac{\partial^2}{\partial\eta_i\,\partial\bar\eta_j}\right|_{\eta=\bar\eta=0} \frac{Z[\eta,\bar\eta]}{Z[0,0]} = \left.\frac{\partial^2}{\partial\eta_i\,\partial\bar\eta_j}\right|_{\eta=\bar\eta=0} e^{\bar\eta A^{-1}\eta} = A^{-1}_{ji},$$

$$\langle \zeta_{j_1}\bar\zeta_{i_1}\;\zeta_{j_2}\bar\zeta_{i_2}\rangle = \left.\frac{\partial^2}{\partial\eta_{i_1}\partial\bar\eta_{j_1}}\,\frac{\partial^2}{\partial\eta_{i_2}\partial\bar\eta_{j_2}}\right|_{\eta=\bar\eta=0} e^{\bar\eta A^{-1}\eta} = A^{-1}_{j_1 i_1}A^{-1}_{j_2 i_2} - A^{-1}_{j_1 i_2}A^{-1}_{j_2 i_1}, \text{ etc.}$$

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 $\langle c_i^\dagger c_j \, c_k^\dagger c_\ell \rangle_0 = \langle c_i^\dagger c_j \rangle_0 \langle c_k^\dagger c_\ell \rangle_0 + \langle c_i^\dagger c_\ell \rangle_0 \langle c_j c_k^\dagger \rangle_0$.

Application. Density-density correlations in a free Fermi gas:

$$\langle \rho(x) \rho(y) \rangle_{\text{conn}} \equiv \langle \rho(x) \rho(y) \rangle_0 - \langle \rho(x) \rangle_0 \langle \rho(y) \rangle_0$$

$$= \langle c^\dagger(x) c(x) \, c^\dagger(y) c(y) \rangle_0 - \langle c^\dagger(x) c(x) \rangle_0 \langle c^\dagger(y) c(y) \rangle_0 = \langle c^\dagger(x) \, c(y) \rangle_0 \, \langle c(x) \, c^\dagger(y) \rangle_0 .$$

$$\langle c^\dagger(x) \, c(y) \rangle_0 = \int \frac{d^dk}{(2\pi)^d} \, e^{ik(x-y)} \langle c_k^\dagger c_k \rangle_0 = \int \frac{d^dk}{(2\pi)^d} \, \frac{e^{ik(x-y)}}{e^{\beta(\varepsilon_k - \mu)} + 1} ,$$

$$\langle c(x) \, c^\dagger(y) \rangle_0 = \int \frac{d^dk}{(2\pi)^d} \, e^{-ik(x-y)} \langle c_k c_k^\dagger \rangle_0 = \int \frac{d^dk}{(2\pi)^d} \, \frac{e^{ik(x-y)}}{e^{-\beta(\varepsilon_k - \mu)} + 1} .$$

$d=1$ and $\beta \to \infty$ $(T \to 0)$: $\langle c^\dagger(x) \, c(y) \rangle_0 = \displaystyle\int_{-k_f}^{k_f} \frac{dk}{2\pi} \, e^{ik(x-y)} = \frac{\sin(k_f(x-y))}{\pi(x-y)}$,

$$\langle c(x) \, c^\dagger(y) \rangle_0 = \int_{|k| > k_f} \frac{dk}{2\pi} \, e^{-ik(x-y)} = \delta(x-y) - \frac{\sin(k_f(x-y))}{\pi(x-y)} .$$

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 $\langle \zeta_i \bar{\zeta}_j \rangle = A^{-1}_{ij}$.

$$\operatorname{Tr} \langle \zeta \bar{\zeta} \rangle \, \delta A = \langle -\bar{\zeta} \, \delta A \cdot \zeta \rangle = \operatorname{Det}^{-1}(A) \, \delta \int e^{-\bar{\zeta} A \zeta}$$

$$= \operatorname{Det}^{-1}(A) \, \delta \operatorname{Det}(A) = \operatorname{Tr} A^{-1} \, \delta A .$$

V.5. Application: high-density electron gas.

Hamiltonian: $$H-\mu N = \int d^3r\, \Psi^\dagger(r)\left(-\frac{\hbar^2}{2m}\Delta-\mu\right)\Psi(r)$$
$$+\frac{1}{2}\int d^3r\int d^3r'\ \hat\rho(r)\,\frac{e^2}{4\pi\varepsilon_0|r-r'|}\,\hat\rho(r'),\qquad \hat\rho(r)=\Psi^\dagger(r)\Psi(r).$$

Partition function: $Z = \mathrm{Tr}\, e^{-\beta(H-\mu N)} = \int \mathcal{D}\bar\psi\,\mathcal{D}\psi\ e^{-S}$,

$$S = \oint_0^\beta d\tau\left\{\int d^3r\ \bar\psi(r,\tau)\left(\frac{\partial}{\partial\tau}-\frac{\hbar^2}{2m}\Delta-\mu\right)\psi(r,\tau)\right.$$
$$\left.+\frac{1}{2}\int d^3r\int d^3r'\ \rho(r,\tau)\,\frac{e^2}{4\pi\varepsilon_0|r-r'|}\,\rho(r',\tau)\right\}.$$

Assume box $Q=[0,L]^3$ with periodic boundary conditions.

To take advantage of translation invariance, use Fourier transform:

$$\psi_{k\omega} = \oint_0^\beta d\tau\int d^3r\ e^{-i(kr-\omega\tau)}\psi(r,\tau);\quad k\in\frac{2\pi}{L}\cdot\mathbb{Z}^3,\ \omega\in\frac{2\pi}{\beta}(\mathbb{Z}+1/2).$$

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 $\tilde V(k)=\dfrac{e^2}{\varepsilon_0|k|^2}$ Fourier transform of Coulomb potential.

Note: Coulomb potential $\notin L^1(\mathbb{R}^3)$ $\rightsquigarrow$ singularity at $k=0$, but $k=0$ is dropped on physical grounds (overall charge neutrality).

Lecture 22.

High-density electron gas: auxiliary-field treatment (Hubbard–Stratonovich transformation)

$$e^{-\frac{1}{2L^3\beta}\sum_{k\omega}\rho_{k\omega}\tilde{V}(k)\,\rho_{-k-\omega}}$$

$$= \int \mathcal{D}\phi \;\; e^{-\frac{1}{L^3\beta}\sum_{k\omega}\left(\frac{e^2}{2}\phi_{k\omega}\tilde{V}(k)^{-1}\phi_{-k-\omega} + ie\,\phi_{k\omega}\,\rho_{-k-\omega}\right)}$$

where $\phi_{-k-\omega} = \overline{\phi_{k\omega}}$ (by choice) and

$$\rho_{k\omega} = \int d\tau \int d^3r \; e^{-i(kr-\omega\tau)}\; \bar{\psi}(r,\tau)\,\psi(r,\tau)$$

$$= \frac{1}{L^3\beta}\sum_{k_1-k_2=k} \;\; \sum_{\omega_1-\omega_2=\omega} \bar{\psi}_{k_2\omega_2}\psi_{k_1\omega_1}\,.$$

Extended action functional:

$$S[\bar{\psi},\psi;\phi] = \frac{e^2}{2L^3\beta}\sum_{k\omega}|\phi_{k\omega}|^2\;\tilde{V}(k)^{-1}$$

$$+ \frac{1}{L^3\beta}\sum_{kk'\omega\omega'}\bar{\psi}_{k\omega}\left(\left(-i\omega + \frac{\hbar^2k^2}{2m} - \mu\right)\delta_{kk'}\,\delta_{\omega\omega'} + ie\,\phi_{k-k',\,\omega-\omega'}\right)\psi_{k'\omega'}\,.$$

Inverse Fourier transform $\rightsquigarrow$ $\phi_{k\omega} = \oint_0^\beta d\tau \int_Q d^3r\; e^{-i(kr-\omega\tau)}\,\phi(r,\tau)\,.$

Action in real space & imaginary time:

$$S[\bar{\psi},\psi;\phi] = \oint_0^\beta d\tau \int_Q d^3r \left\{ \frac{\varepsilon_0}{2}\,(\nabla\phi)^2 + \bar{\psi}\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right)\psi \right\}.$$

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 ($\rightsquigarrow$ interpretation of ϕ as a (fictitious) electric scalar potential).

Integrate out the electron field:

$$Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \; e^{-S[\bar{\psi},\psi]} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \int \mathcal{D}\phi \; e^{-S[\bar{\psi},\psi;\phi]}$$

$$= \int \mathcal{D}\phi \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \; e^{-\oint d\tau \int d^3r \left(\frac{\varepsilon_0}{2} (\nabla\phi)^2 + \bar{\psi}\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right)\psi \right)}$$

$$= \int \mathcal{D}\phi \; e^{-\frac{\varepsilon_0}{2}\oint d\tau \int d^3r (\nabla\phi)^2} \mathrm{Det}\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right) = \int \mathcal{D}\phi \; e^{-S_{\mathrm{eff}}[\phi]}$$

with effective action

$$S_{\mathrm{eff}}[\phi] = \frac{\varepsilon_0}{2}\oint d\tau \int d^3r (\nabla\phi)^2 - \mathrm{Tr}\ln\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right).$$

Inspection shows that this effective action has no extema away from $\phi = 0$.

To expand S_{eff} around $\phi = 0$, use the identity (if $\|A^{-1}B\| < 1$)

$$-\mathrm{Tr}\ln(A - B) = -\mathrm{Tr}\ln\left(A(1 - A^{-1}B)\right) = -\mathrm{Tr}\ln A - \mathrm{Tr}\ln(1 - A^{-1}B)$$
$$= -\ln \mathrm{Det} A + \sum_{n=1}^{\infty} \frac{1}{n}\mathrm{Tr}(A^{-1}B)^n$$

for $A = \frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu \equiv G_0^{-1}$ and $B = -ie\phi$.

Then $-\mathrm{Tr}\ln\left(\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\Delta - \mu + ie\phi\right) = \ln \mathrm{Det}\, G_0 + \sum_{n=1}^{\infty} \frac{(-ie)^n}{n}\mathrm{Tr}(G_0\phi)^n.$

The term linear in ϕ vanishes because G_0 is constant on the diagonal and $\int d^3r\, \phi \propto \phi_{k=0} = 0$ by overall charge neutrality. The quadratic term:

$$\mathrm{Tr}(G_0\phi\, G_0\phi) = \frac{1}{(L^3\beta)^2}\sum_{kk'\omega\omega'} G_0(k,\omega)\,\phi_{k-k',\omega-\omega'}\,G_0(k',\omega')\,\phi_{k'-k,\omega'-\omega}$$
$$\equiv \frac{1}{L^3\beta}\sum_{k\omega} \Pi(k,\omega)\,\phi_{k\omega}\phi_{-k-\omega}.$$

Altogether we have $S_{\mathrm{eff}} = \frac{1}{2L^3\beta}\sum_{k\omega}\left(\varepsilon_0|k|^2 - e^2\Pi(k,\omega)\right)|\phi_{k\omega}|^2 + \ldots$

where $\Pi(q,\omega) = \frac{1}{L^3\beta}\sum_{k\varepsilon} G_0(k,\varepsilon)\,G_0(k+q,\varepsilon+\omega)$ is the polarization operator.

Its appearance suppresses fluctuations of the electric scalar potential $\phi_{k\omega}$ at long wave lengths (or small wave number k) and small frequencies ω. This is seen as follows.

To get a closed expression for $\Pi(q,\omega)$,

$$\Pi(q,\omega) = \frac{1}{L^3\beta} \sum_{k\xi} \left(-i\xi + \varepsilon_k - \mu\right)^{-1} \left(-i(\omega+\xi) + \varepsilon_{k+q} - \mu\right)^{-1},$$

use the identities $a^{-1} b^{-1} = (b-a)^{-1}(a^{-1} - b^{-1})$ and

$$\frac{2\pi i}{-\beta} \sum_{\xi \in \frac{2\pi i}{\beta}(\mathbb{Z}-\frac{1}{2})} f(\xi) = \oint \frac{f(z)\, dz}{e^{\beta z}+1} .$$ Then

$$\Pi(q,\omega) = \frac{1}{L^3} \sum_k \frac{-1}{2\pi i} \int \frac{dz}{e^{\beta z}+1} \cdot \frac{1}{\varepsilon_{k+q} - i\omega - \varepsilon_k} \left(\frac{1}{-z + \varepsilon_k - \mu} - \frac{1}{-z - i\omega + \varepsilon_{k+q} - \mu} \right)$$

$$= \frac{1}{L^3} \sum_k \frac{n_f(\varepsilon_{k+q} - i\omega) - n_f(\varepsilon_k)}{\varepsilon_{k+q} - i\omega - \varepsilon_k} ,$$

where $n_f(\varepsilon) = \left(e^{\beta(\varepsilon-\mu)} + 1\right)^{-1}$ is the Fermi-Dirac distribution function.

Discussion of the static limit $(\omega \to 0)$ and long wave lengths $(|q|$ small$)$:

$$\Pi(q,0) = \frac{1}{L^3} \sum_k \frac{n_f(\varepsilon_{k+q}) - n_f(\varepsilon_k)}{\varepsilon_{k+q} - \varepsilon_k} \overset{q \to 0}{\approx} \frac{1}{L^3} \sum_k n_f'(\varepsilon_k) = \int d\varepsilon\, \nu(\varepsilon)\, n_f'(\varepsilon) = -\nu(\varepsilon_f) .$$

Effective interaction (later interpreted as 4-print vertex function)

$$V_{eff}(q,\omega) = \frac{V(q)}{1 - V(q)\Pi(q,\omega)} .$$ Static limit:

$$V_{eff}(q,0) = \frac{1}{V(q)^{-1} - \Pi(q,0)} = \frac{1}{\left(\frac{e^2}{\varepsilon_0} \cdot \frac{1}{|q|^2}\right)^{-1} + \nu_F} \sim \frac{1}{|q|^2 + \lambda^{-2}}, \quad \lambda^{-2} = \nu_F \cdot \frac{e^2}{\varepsilon_0} .$$

$\lambda =$ screening length

Lecture 23.

VI. 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, $\operatorname{div} \vec{A} = 0$) to eliminate the unphysical degrees of freedom in $\vec{A}$.

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

VI.1 Canonical quantization (of the E.M. field in vacuum)

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

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

2. Symplectic structure / form α

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

$\operatorname{rot}^{-1} B = A$ 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 $\int d^3r \, D \cdot (A - A') = \int d^3r \, D \cdot \operatorname{grad} f \overset{\nearrow}{=} - \int d^3r \, f \operatorname{div} D = 0$.

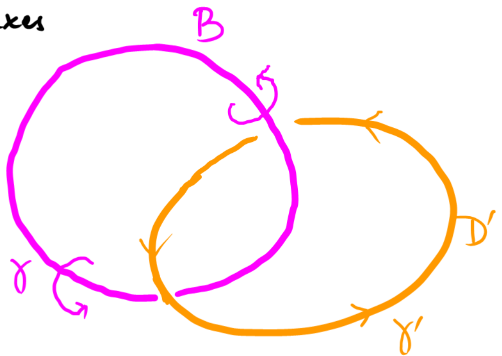
D assumed to vanish on boundary of domain

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

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

For special configurations where D' and B are confined to the interior of narrow tubes γ' and γ, this becomes $\int d^3r \, D' \cdot \operatorname{rot}^{-1} B = \Phi_{D'} \Phi_B \, G(\gamma, \gamma')$ 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 $H = \int d^3r \left(\frac{|D|^2}{2\varepsilon_0} + \frac{|B|^2}{2\mu_0} \right)$, the symplectic form α gives the proper equations of motion (Maxwell in vacuum).

3. Complex structure J.

As before (L09: harmonic oscillator) 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 $D^\lambda_\perp\Big|_{\partial\mathcal{U}} = 0$, 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 $(D_t, B_t) = (D^\lambda\cos(\omega_\lambda t), B^\lambda \sin(\omega_\lambda t))$ is a solution of Maxwell's equations, and so is $(D_t, B_t) = (-D^\lambda \sin(\omega_\lambda t), B^\lambda\cos(\omega_\lambda t))$.

The normal modes $(D^\lambda, 0)$ and $(0, B^\lambda)$ span the two-dimensional space W_λ. The complex structure J restricted to W_λ is given by

$$J(D^\lambda, 0) = (0, B^\lambda) = \left(0, -\frac{\operatorname{rot} D^\lambda}{\omega_\lambda \varepsilon_0}\right)$$

$$\text{and} \quad J(0, B^\lambda) = (-D^\lambda, 0) = \left(\frac{\operatorname{rot} B^\lambda}{\omega_\lambda \mu_0}, 0\right).$$

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

Exercise. $J^2 = -1$, and J preserves α.

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

$$g\big((D^\lambda, B^\lambda), (D^\lambda, B^\lambda)\big) = \alpha\big((D^\lambda, B^\lambda), J(D^\lambda, B^\lambda)\big) = \frac{2}{\omega_\lambda} H(D^\lambda, B^\lambda) \geqslant 0. \ ✓$$

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

$$V_\lambda = \mathbb{C}\cdot e_\lambda, \quad e_\lambda = \frac{1}{\sqrt{2}}\Big((D_0^\lambda, 0) + iJ(D_0^\lambda, 0)\Big) = \frac{1}{\sqrt{2}}(D_0^\lambda, iB_0^\lambda),$$

$$V_\lambda^* \cong \tilde{V}_\lambda = \mathbb{C}\cdot\tilde{e}_\lambda, \quad \tilde{e}_\lambda = \frac{1}{\sqrt{2}}\Big((D_0^\lambda, 0) - iJ(D_0^\lambda, 0)\Big) = \frac{1}{\sqrt{2}}(D_0^\lambda, -iB_0^\lambda).$$

normalization $H(D_0^\lambda, 0) = \frac{1}{2}\hbar\omega_\lambda$.

Photon creation operators $a_\lambda^+ = \mu(e_\lambda)$, annihilation ops $a_\lambda = \delta(\tilde{e}_\lambda)$.

Fock space $S(V)$, $V = \oplus_\lambda V_\lambda$. Hermitian scalar product $\rightsquigarrow$ $(a_\lambda^+)^\dagger = a_\lambda$.

Mode expansion. $\hat{D}(r) = \frac{1}{\sqrt{2}} \sum_\lambda D_0^\lambda(r) \left(a_\lambda^+ + a_\lambda\right),$

$$\hat{B}(r) = \frac{1}{\sqrt{2}i} \sum_\lambda B_0^\lambda(r) \left(a_\lambda^+ - a_\lambda\right) = \frac{i}{\sqrt{2}} \sum_\lambda \frac{\mathrm{rot}\, D_0^\lambda(r)}{\omega_\lambda \varepsilon_0} \left(a_\lambda^+ - a_\lambda\right).$$

Insert into the expression for the Hamiltonian $\rightsquigarrow$ $\hat{H} = \frac{1}{2} \sum_\lambda \hbar\omega_\lambda \left(a_\lambda^+ a_\lambda + a_\lambda a_\lambda^+\right).$

For more details, see my lectures on Advanced Quantum Mechanics.

A summary/comparison of canonical quantization of bosons vs. fermions is appended at the end of L23.

VI.2 Coherent-state path integral for bosons

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

Resolution of unity: $1_{S(V)} = \int T_z |\mathrm{vac}\rangle\langle\mathrm{vac}| T_z^{-1}.$

$T_z = \exp \sum_j \left(a_j^+ z_j - \bar{z}_j a_j\right) \equiv e^{z a^+ - \bar{z} a}$ unitary operator.

$T_u T_v = T_{u+v}\, e^{-\omega(u,v)/2}, \quad \omega(u,v) = \bar{u} v - u \bar{v} \in i\mathbb{R}.$

$\mathrm{Tr}\, e^{-\mathcal{H}(a^+,a)} = \lim_{M\to\infty} \int e^{-S}$ where

normal-ordered

$$S = \sum_{n=1}^{M} \Big(\tfrac{1}{2} \bar{z}(n) z(n) + \tfrac{1}{2} \bar{z}(n+1) z(n+1) - \bar{z}(n+1) z(n) + \tfrac{\beta}{M} \mathcal{H}\left(\bar{z}(n+1), z(n)\right)\Big).$$

Continuum limit: $z(n) \longrightarrow \varphi(\tau)$,
$\bar{z}(n) \longrightarrow \bar{\varphi}(\tau)$.

Periodic boundary conditions $\varphi(\tau) = \varphi(\tau+\beta)$, $\bar{\varphi}(\tau) = \bar{\varphi}(\tau+\beta)$.

$$S = \oint_0^\beta d\tau \left(\bar{\varphi} \frac{\partial}{\partial\tau} \varphi + \mathcal{H}(\bar{\varphi}, \varphi)\right) \quad \text{(imaginary time)}.$$

Real time: $S = \oint_0^T dt \left(\bar{\varphi} \frac{\partial}{\partial t} \varphi + \frac{i}{\hbar} \mathcal{H}(\bar{\varphi}, \varphi)\right).$

Review of Field Quantization

A field here is a mapping
$$f : \text{space} \times \text{time} \longrightarrow \text{target space}$$
$$(r,t) \longmapsto f(r,t)$$

Examples: Dirac field (spinor)

electomagnetic gauge field (vector)

Higgs field (scalar).

choice of vacuum

Quantization (fixed time t):
$$f = f^{+} + f^{-}$$

creates particles 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

$$B : W \otimes W \longrightarrow \mathbb{C}, \qquad B(v_1 + \varphi_1 , v_2 + \varphi_2) = \begin{cases} \varphi_1(v_2) + \varphi_2(v_1) & \text{fermions} \\ \varphi_1(v_2) - \varphi_2(v_1) & \text{bosons} \end{cases}$$

2\. Fock algebra (operators, still abstract) $=$

associative algebra generated by $W \oplus \mathbb{C}$

subject to the relations $w w' + \epsilon\, w' w = B(w,w') \cdot 1$ unit element (central)

fermions: $\epsilon = +1$, CAR, Clifford algebra $Cl(W,B)$

bosons: $\epsilon = -1$, CCR, Weyl algebra $W(W,B)$

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

$W(W_{\mathbb{R}}, B)$ 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: $B(Jw, Jw') = B(w,w')$.

Remark: a choice of complex structure determines a choice of vacuum (see below).

5. J-eigenspaces: $E_{+i}(J) \equiv \mathcal{F}^- \rightsquigarrow$ annihilation operators : $f^-|\mathrm{vac}\rangle = 0$

$E_{-i}(J) \equiv \mathcal{F}^+ \rightsquigarrow$ creation operators : $f^+|\mathrm{vac}\rangle \neq 0$

Note: $B(\mathcal{F}^-,\mathcal{F}^-) = 0 = B(\mathcal{F}^+,\mathcal{F}^+)$: $\mathcal{F}^\pm$ "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 $\langle \cdot,\cdot \rangle_V$.

Language: $\Lambda(\mathcal{F}^+) \subset \mathrm{Cl}(W,B)$ exterior algebra

$S(\mathcal{F}^+) \subset \mathcal{W}(W,B)$ symmetric algebra

Representation of Fock algebra on Fock space $\longrightarrow$ later.

Example. single harmonic oscillator mode

0. $V = \mathbb{C}\cdot a^+ \simeq \mathbb{C}$, $\langle a^+, a^+\rangle = 1$.

$V^* = \mathbb{C}\cdot a \simeq \mathbb{C}$; a is basis vector dual to a^+, i.e. $a(a^+) = 1$.

1. $W = \mathrm{span}_{\mathbb{C}}\{a, a^+\} \simeq \mathbb{C}^2$.

$B(v_1 a^+ + u_1 a,\ v_2 a^+ + u_2 a) = u_1 v_2 - v_1 u_2$.

2. Weyl algebra $\mathcal{W}(W,B)$ = algebra of polynomials in a, a^+ with relation $a a^+ - a^+ a = 1$.

3. Identify $a \equiv \langle a^+, \cdot \rangle_V$.

position & momentum

$$W_{\mathbb{R}} = \mathrm{span}_{\mathbb{R}}\left\{ \frac{a+a^+}{\sqrt{2}}, \frac{a-a^+}{\sqrt{2}\,i} \right\} = \mathrm{span}_{\mathbb{R}}\{q,p\}.$$

4. Standard complex structure J:

$$\begin{matrix} Ja = ia \\ Ja^+ = -ia^+ \end{matrix} \iff \begin{matrix} Jq = -p \\ Jp = +q \end{matrix}$$

Note

$J^2 = -1$ ✓

& preserves B ✓

Physical meaning: J = phase flow $\phi_{t=T/4}$

$V = E_{-i}(J) = \mathcal{F}^+$

$V^* = E_{+i}(J) = \mathcal{F}^-$

5. Fock space $= S(\mathcal{F}^+) = S(V)$

with $\langle (a^+)^m, (a^+)^n \rangle_{S(V)} = \delta_{mn}\cdot n!$

Lecture 24.

Coherent-state path integral for bosons (cont'd).

Recall $\operatorname{Tr} e^{-iT\hat{H}/\hbar} = \int \mathcal{D}\bar\varphi\, \mathcal{D}\varphi\; e^{-S}$

$$S = \oint dt \left(\bar\varphi \frac{\partial}{\partial t}\varphi + \frac{i}{\hbar} H(\bar\varphi, \varphi)\right).$$

Phase-space path integral:

Put $q = \frac{\ell}{\sqrt2}(\varphi + \bar\varphi)$ and $p = \frac{\hbar}{\sqrt2 i\ell}(\varphi - \bar\varphi)$.

Then $\oint dt\; \bar\varphi \frac{\partial}{\partial t}\varphi = -\frac{i}{\hbar}\oint dt\; p \frac{\partial}{\partial t} q$

and $\operatorname{Tr} e^{-iT\hat{H}/\hbar} = \int \mathcal{D}q\, \mathcal{D}p\; e^{\frac{i}{\hbar}\oint (p\,dq - H\,dt)}$.

Poincaré–Cartan (CM)

Generalizations exist to, e.g., spin systems, where phase space is a symplectic manifold (with Kähler structure).

Reduction to the position-space path integral

is possible for Hamiltonians of the form $H = \frac{p^2}{2m} + V(q)$.

Indeed, $\int \mathcal{D}p\; e^{\frac{i}{\hbar}\oint dt\,(p\dot q - \frac{p^2}{2m})} = e^{+\frac{i}{\hbar}\oint dt\, \frac{m}{2}\dot q^2}$, so

$$\operatorname{Tr} e^{-iT\hat{H}/\hbar} = \int \mathcal{D}q\; e^{\frac{i}{\hbar}\oint dt\,(\frac{m}{2}\dot q^2 - V(q))} = \int \mathcal{D}q\; e^{\frac{i}{\hbar}\oint \mathcal{L}\, dt}.$$

Turn to the electromagnetic field.

Hamiltonian function $H = \int d^3r \left(\frac{|D|^2}{2\varepsilon_0} + \frac{|B|^2}{2\mu_0}\right)$,

Lagrangian function $\mathcal{L} = \int d^3r \left(\frac{|D|^2}{2\varepsilon_0} - \frac{|B|^2}{2\mu_0}\right)$,

$\int \mathcal{L}\,dt = -\frac14\sqrt{\frac{\varepsilon_0}{\mu_0}}\int d^4x\; F_{\mu\nu}F^{\mu\nu}$.

Quantum electrodynamics.

$$S_{QED} = \int d^4x\; \bar\psi\left(\gamma^\mu\left(\frac{\hbar}{i}\frac{\partial}{\partial x^\mu} - eA_\mu\right) + mc\right)\psi - \frac14\sqrt{\frac{\varepsilon_0}{\mu_0}}\int d^4x\; F_{\mu\nu}F^{\mu\nu},$$

E.M. field strength $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. Note $-\frac{c}{4}\sqrt{\frac{\varepsilon_0}{\mu_0}}F_{\mu\nu}F^{\mu\nu} = \frac{\varepsilon_0\vec E^2}{2} - \frac{\vec B^2}{2\mu_0}$.

Lagrange density

$\left[\sqrt{\frac{\varepsilon_0}{\mu_0}}\right] = \frac{\text{charge}^2}{\text{action}} = \frac{\text{current}}{\text{voltage}} = $ conductance.

Fine structure constant $\alpha = \frac12\frac{e^2}{h}\sqrt{\frac{\varepsilon_0}{\mu_0}}^{-1} = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137}$.

Exercise. $0 = \frac{\delta}{\delta A_\nu}S_{QED} \Longrightarrow \sqrt{\frac{\varepsilon_0}{\mu_0}}\,\partial_\mu F^{\mu\nu} = J^\nu = e\bar\psi\gamma^\nu\psi$.

(inhomogeneous Maxwell eqns)

Scale the gauge field: $a_\mu = \hbar^{-1/2}\left(\frac{\varepsilon_0}{\mu_0}\right)^{1/4} A_\mu$. Let $f_{\mu\nu} = \partial_\mu a_\nu - \partial_\nu a_\mu$.

Then $\mathrm{FPI} = \int \mathcal{D}a \; e^{-\frac{i}{4}\int d^4x\, f_{\mu\nu} f^{\mu\nu}} \cdot \int \mathcal{D}\bar\psi \mathcal{D}\psi \; e^{\int d^4x\, \bar\psi(\gamma^\mu \partial_\mu + imc/\hbar)\psi}$

$\cdot\, e^{-2i\sqrt{\alpha}\int d^4x\, a_\mu \bar\psi \gamma^\mu \psi}$ ← interaction vertex

Advantage: relativistic covariance & computational simplicity

Free fields: two-point function. Gaussian integral over real variables:

$$\ln \int d^N\phi \; e^{-\frac{1}{2}\sum_{kl} \phi_k (B_{kl} + \underset{\text{"source"}}{j_{kl}}) \phi_l} = \ln \mathrm{Det}^{-1/2}\left((B+j)/2\pi\right) \equiv \ln Z(j) .$$

$$\left.\frac{\partial}{\partial j_{kl}}\right|_{j=0} \text{ gives } Z(0)^{-1} \int d^N\phi \left(-\tfrac{1}{2}\phi_k\phi_l\right) e^{-\frac{1}{2}\phi^t B \phi} = -\frac{1}{2}\left.\frac{\partial}{\partial j_{kl}}\right|_{j=0} \mathrm{Tr} \ln(1 + B^{-1}j) = -\frac{1}{2} {B^{-1}}_{lk} .$$

$$\text{Hence } Z(0)^{-1} \int d^N\phi \; \phi_l \phi_k \; e^{-\frac{1}{2}\phi^t B\phi} \overset{\text{def}}{=} \langle \phi_l \phi_k \rangle = {B^{-1}}_{lk} .$$

Photon propagator (first attempt).

$$\exp\left(\tfrac{i}{\hbar} S\right) = \exp\left(-\frac{i}{4\hbar}\sqrt{\frac{\varepsilon_0}{\mu_0}} \int d^4x\, F_{\mu\nu}F^{\mu\nu}\right)$$

$$\int d^4x\, F_{\mu\nu}F^{\mu\nu} = \int d^4x\, (\partial_\mu A_\nu - \partial_\nu A_\mu)(\partial^\mu A^\nu - \partial^\nu A^\mu)$$

$\Box = \partial_\mu \partial^\mu$ d'Alembert operator

$$= 2\int d^4x\, (\partial_\mu A_\nu) F^{\mu\nu} = -2\int d^4x\, A_\nu (\delta^\nu_\mu \Box - \partial^\nu \partial_\mu) A^\mu .$$

Problem! The operator $A^\nu \mapsto (\delta^\nu_\mu \Box - \partial^\nu\partial_\mu) A^\mu$ has a non-trivial kernel.

Indeed, for $A^\mu(x) = k^\mu e^{ik\cdot x}$ (where $k \cdot x = \eta_{\mu\nu} k^\mu x^\nu = \mathbf{k}\cdot\mathbf{r} - \omega t$) one obtains

$$(\delta^\nu_\mu \Box - \partial^\nu\partial_\mu) A^\mu = -(\delta^\nu_\mu k\cdot k - k^\nu k_\mu) k^\mu e^{ik\cdot x} = -(k\cdot k - k\cdot k) k^\nu e^{ik\cdot x} = 0 .$$

By consequence, the inverse of $A^\nu \mapsto (\delta^\nu_\mu \Box - \partial^\nu\partial_\mu) A^\mu$ does not exist.

<u>Reason</u>: $F_{\mu\nu}$ invariant under gauge transformations $A_\mu \longrightarrow A_\mu + \partial_\mu f$.

Gauge fixing/averaging. — Recall Coulomb gauge $\mathrm{div}\vec{A} = 0$, $\phi = 0$.

— The Lorenz gauge $\partial_\mu A^\mu = 0$ is Lorentz-invariant.

Ludvig Lorenz, 1867 (Danish)

Hendrik Lorentz (Dutch, Leiden, Physics Nobel Prize 1902: Zeeman effect)

Feynman–t'Hooft gauges: add $-\frac{1}{2\beta}\sqrt{\frac{\varepsilon_0}{\mu_0}} \int d^4x\, (\partial_\mu A^\mu)^2$ to action functional.

$$\text{Feynman gauge } (\beta = 1):\; S_{\mathrm{E.M.}} = -\frac{1}{4}\sqrt{\frac{\varepsilon_0}{\mu_0}} \int d^4x \left(F_{\mu\nu}F^{\mu\nu} + 2(\partial_\mu A^\mu)^2\right)$$

$$= \frac{1}{2}\sqrt{\frac{\varepsilon_0}{\mu_0}} \int d^4x\, A_\nu \Box A^\nu .$$

Info. The issue of gauge fixing is an open problem (← Gribov ambiguities) in non-Abelian gauge theories.

Photon propagator in Landau gauge.

Recall $\exp\left(\frac{i}{\hbar} S_{\text{E.M.}}\right) = \exp\left(-\frac{i}{4\hbar}\sqrt{\frac{\varepsilon_0}{\mu_0}}\int d^4x\, F_{\mu\nu}F^{\mu\nu}\right)$ and

$$\frac{1}{4}\int d^4x\, F_{\mu\nu}F^{\mu\nu} = -\frac{1}{2}\int d^4x\, A_\nu\left(\delta^\nu_\mu \Box - \partial^\nu\partial_\mu\right)A^\mu .$$

Fourier transform to energy-momentum space:

$$\frac{1}{4}\int d^4x\, F_{\mu\nu}F^{\mu\nu} = +\frac{1}{2}\int \frac{d^4q}{(2\pi)^4}\, A_\mu(q)\left(\eta^{\mu\nu}q^2 - q^\mu q^\nu\right)A_\nu(-q) .$$

Lorenz gauge condition: $q^\mu A_\mu(q) = 0$. In the subspace singled out by this constraint the non-invertible quadratic form

$$\Pi^{\mu\nu}(q) = \eta^{\mu\nu}q^2 - q^\mu q^\nu$$

has an inverse (called the photon propagator in Landau gauge)

$$\Pi_{\mu\nu}(q) = \frac{1}{q^4}\left(\eta_{\mu\nu}q^2 - q_\mu q_\nu\right).$$

vanishes on the solution space of the Lorenz gauge condition.

CHECK: $\Pi^{\mu\nu}(q)\,\Pi_{\nu\lambda}(q) = \delta^\mu_\lambda - q^\mu q_\lambda/q^2$ (✓)

Photon propagator in real space-time:

$$\langle A_\mu(x)\, A_\nu(y)\rangle = \int \frac{d^4q}{(2\pi)^4}\,\frac{1}{q^4}\left(\eta_{\mu\nu}q^2 - q_\mu q_\nu\right)e^{iq\cdot(x-y)} .$$

OUTLOOK: QFT-2 (WS 20/21)

- perturbation theory: Feynman graphs (→ QED)
- spontaneous symmetry breaking: Goldstone modes
- Anderson-Higgs mechanism: theory of superconductivity
- duality transformations (strong coupling ⟷ weak coupling)
- renormalization group: ideas and practice