1 Classical and Quantum Mechanics

To familiarise ourselves with the basics, let us review some elements of classical and quantum mechanics. Then we shall discuss some problems of combining quantum mechanics with special relativity.

1.1 Classical Mechanics

Consider a classical non-relativistic particle in a potential. Described by position variables $q^i(t)$ and action functional $S[q]$ [1] [2]

$$S[q] = \int_{t_1}^{t_2} dt\, L(q^i(t), \dot{q}^i(t), t) \tag{1.1}$$

A typical Lagrangian function is

$$L(\vec{q}, \dot{\vec{q}}) = \tfrac{1}{2} m \dot{\vec{q}}^2 - V(\vec{q}). \tag{1.2}$$

with mass m and $V(q)$ external potential.

A classical path extremises (minimises) the action S. Determine saddle-point $\delta S = 0$ by variation of the action[3]

$$\begin{aligned} \delta S &= \int_{t_1}^{t_2} dt \left(\delta q^i(t) \frac{\partial L}{\partial q^i} + \delta \dot{q}^i(t) \frac{\partial L}{\partial \dot{q}^i} \right) \\ &= \int_{t_1}^{t_2} dt\, \delta q^i(t) \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} \right) + \int_{t=t_1}^{t=t_2} d \left(\delta q^i(t) \frac{\partial L}{\partial \dot{q}^i} \right) \overset{!}{=} 0 \end{aligned} \tag{1.3}$$

First term is equation of motion (Euler–Lagrange)

$$\frac{\delta S}{\delta q^i(t)} = \frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} = 0. \tag{1.4}$$

Second term due to partial integration is boundary e.o.m., usually ignore.[4]

Example. Harmonic oscillator (free particle for $\omega = 0$)

$$L(\vec{q}, \dot{\vec{q}}) = \tfrac{1}{2} m \dot{\vec{q}}^2 - \tfrac{1}{2} m \omega^2 \vec{q}^2, \qquad -m(\ddot{\vec{q}} + \omega^2 \vec{q}) = 0. \tag{1.5}$$

[1] L is often time-independent: $L(q^i, \dot{q}^i, t) = L(q^i, \dot{q}^i)$.

[2] A single time derivative $\dot{q}^i$ usually suffices.

[3] Einstein summation convention: there is an implicit sum over all values for pairs of equal upper/lower indices.

[4] Usually fix position $q_i(t_k) = \text{const.}$ (Dirichlet) or momentum $\partial L / \partial \dot{q}^i(t_k) = 0$ (Neumann) at boundary.

1.2 Hamiltonian Formulation

The Hamiltonian framework is the next step towards canonical quantum mechanics.

Define conjugate momentum p_i as[5]

$$p_i = \frac{\partial L}{\partial \dot{q}^i} \tag{1.6}$$

and solve for $\dot{q}^i = \dot{q}^i(q, p, t)$.[6] Define phase space as (q^i, p_i).

Lagrangian function $L(q, \dot{q}, t)$ replaced by Hamiltonian function $H(q, p, t)$ on phase space. Define $H(q^i, p_i, t)$ as Legendre transformation of L

$$H(q, p, t) = p_i \dot{q}^i(q, p, t) - L(q, \dot{q}(q, p, t), t). \tag{1.7}$$

Let us express e.o.m. through H. General variation reads

$$\delta H = \delta p_i \dot{q}^i - \delta q^i \frac{\partial L}{\partial q^i} \tag{1.8}$$

where we substituted definition of momenta p_i twice. Use Euler–Lagrange equation and momenta to simplify further

$$\delta H = \delta p_i \dot{q}^i - \delta q^i \dot{p}_i. \tag{1.9}$$

Now, Hamiltonian e.o.m. $\dot{q}^i = \partial H / \partial p_i$ and $\dot{p}_i = -\partial H / \partial q^i$.

Introduce Poisson brackets for functions f, g on phase space

$$\{f, g\} := \frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i}\,. \tag{1.10}$$

Express time evolution for phase space functions $f(p, q, t)$ [7]

$$\frac{df}{dt} = \frac{\partial f}{\partial t} - \{H, f\}. \tag{1.11}$$

Works well for $f = q^i$ and $f = p_i$.

Example. Harmonic oscillator

$$\vec{p} = m\dot{\vec{q}}, \qquad H = \vec{p}\cdot\dot{\vec{q}} - \frac{m}{2}\dot{\vec{q}}^2 + \frac{m\omega^2}{2}\vec{q}^2 = \frac{1}{2m}\vec{p}^2 + \frac{m}{2}\omega^2\vec{q}^2. \tag{1.12}$$

Hamiltonian equations of motion

$$\dot{\vec{q}} = -\{H, \vec{q}\} = \frac{\partial H}{\partial \vec{p}} = \frac{1}{m}\vec{p}, \quad \dot{\vec{p}} = -\{H, \vec{p}\} = -\frac{\partial H}{\partial \vec{q}} = -m\omega^2\vec{q}. \tag{1.13}$$

[5] This is a choice, could also use different factors or notations.
[6] Suppose the equation can be solved for $\dot{q}$.
[7] The Hamiltonian H is a phase space function.

Convenient change of variables

$$\vec{a} = \frac{1}{\sqrt{2m\omega}} \left(m\omega\vec{q} + i\vec{p} \right), \qquad \vec{a}^* = \frac{1}{\sqrt{2m\omega}} \left(m\omega\vec{q} - i\vec{p} \right), \tag{1.14}$$

with new Poisson brackets

$$\{f, g\} = -i \frac{\partial f}{\partial a^i} \frac{\partial g}{\partial a_i^*} + i \frac{\partial f}{\partial a_i^*} \frac{\partial g}{\partial a^i} \,. \tag{1.15}$$

Separated first-order time evolution for $\vec{a}, \vec{a}^\dagger$

$$H = \omega\vec{a}^\dagger\vec{a}, \qquad \dot{\vec{a}} = -i\omega\vec{a}, \quad \dot{\vec{a}}^\dagger = +i\omega\vec{a}^\dagger. \tag{1.16}$$

1.3 Quantum Mechanics

In canonical quantisation classical objects are replaced by elements of linear algebra:

- The state (q^i, p_i) becomes a vector $|\psi\rangle$ in a Hilbert space V.
- A phase space function f becomes a linear operator F on V.
- Poisson brackets $\{f, g\}$ become commutators $-i\hbar^{-1}[F, G]$.[8]

State equation of motion (Schrödinger), wave equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H|\psi(t)\rangle. \tag{1.17}$$

Probabilistic role of wave function: $|\langle\phi|\psi\rangle|^2$ is probability. Requires:

- $\langle\psi|\psi\rangle$ is positive.
- $\langle\psi|\psi\rangle$ can be normalised to 1 by scaling $|\psi\rangle$.
- $\langle\psi|\psi\rangle$ is conserved

$$\frac{d}{dt}\langle\psi|\psi\rangle = (i\hbar)^{-1}\langle\psi|(H - H^\dagger)|\psi\rangle = 0. \tag{1.18}$$

  Hamiltonian is hermitian (self-adjoint). Unitary time evolution: $|\psi(t_2)\rangle = U(t_2, t_1)|\psi(t_1)\rangle$.
- $\langle\psi|F|\psi\rangle$ is expectation value of operator F. Obeys classical time evolution.

Example. Harmonic oscillator, free particle.

Momentum operator and Hamiltonian[9]

$$\vec{p} = -i\hbar \frac{\partial}{\partial\vec{q}}, \quad [q^i, p_j] = i\hbar\delta^i_j, \quad H = -\frac{\hbar^2}{2m} \left(\frac{\partial}{\partial\vec{q}} \right)^2 + \frac{m\omega^2}{2} \vec{q}^2. \tag{1.19}$$

[8]Cannot always be translated literally, but up to simpler terms.

[9]Note: $\vec{p} = -i\hbar\vec{\partial}\vec{q}$ vs. $E = +i\hbar\partial_t$. On wave function $|\psi\rangle = \int d^d\vec{q}\,\psi(\vec{q}, t)|\vec{q}\rangle$, however: $\vec{p}|\psi\rangle = +i\hbar \int d^d\vec{q}\,\vec{\partial}\psi(\vec{q}, t)|\vec{q}\rangle$ and $E|\psi\rangle = +i\hbar \int d^d\vec{q}\,\partial_t\psi(\vec{q}, t)|\vec{q}\rangle$

Free particle: momentum eigenstate (Fourier transforms)

$$|\vec{p}\rangle = \int d^d\vec{q}\, e^{-i\hbar^{-1}\vec{p}\cdot\vec{q}}|\vec{q}\rangle, \qquad |\vec{q}\rangle = \int \frac{d^d\vec{p}}{(2\pi\hbar)^d}\, e^{i\hbar^{-1}\vec{p}\cdot\vec{q}}|\vec{p}\rangle. \tag{1.20}$$

$|\vec{p}\rangle$ is energy eigenstate with $E = \vec{p}^{\,2}/2m$.

Harmonic oscillator: use operators a^i and $a_i^\dagger$

$$\vec{a} = \frac{1}{\sqrt{2m\omega}}\left(m\omega\vec{q} + \hbar\frac{\partial}{\partial\vec{q}}\right), \quad \vec{a}^\dagger = \frac{1}{\sqrt{2m\omega}}\left(m\omega\vec{q} - \hbar\frac{\partial}{\partial\vec{q}}\right), \tag{1.21}$$

with commutators

$$[a^i, a_j^\dagger] = \hbar\delta^i_j. \tag{1.22}$$

Quantum Hamiltonian has extra vacuum energy $E_0 = \frac{1}{2}d\hbar\omega$

$$H = \tfrac{1}{2}\omega a^i a_i^\dagger + \tfrac{1}{2}\omega a_i^\dagger a^i = \omega\vec{a}^\dagger\vec{a} + \tfrac{1}{2}d\hbar\omega = \omega\vec{a}^\dagger\vec{a} + E_0. \tag{1.23}$$

- Can add any E_0 to Hamiltonian. No effect. E_0 is irrelevant. Unless: E couples to something else (e.g. gravity).
- Same effect as adding $i\alpha(\vec{q}\cdot\vec{p} - \vec{p}\cdot\vec{q})$ to H.[10] Classically invisible. Quantum energy shift $\Delta E_0 = -d\alpha\hbar$. Quantum ordering ambiguity. Harmless, affects trivial E_0.
- Quantum theory does as it pleases, e.g. introduce/shift E_0. Best to consider all allowable terms in the first place.

Construct spectrum: Start from vacuum state $|0\rangle$ to be annihilated by $\vec{a}$ (has energy $E = E_0$, but irrelevant)

$$a^i|0\rangle = 0. \tag{1.24}$$

Add excitations $n_i \geq 0$ and normalise state $\langle\vec{n}|\vec{n}\rangle = 1$

$$|\vec{n}\rangle = \left(\prod_{i=1}^{d}\frac{(a_i^\dagger)^{n_i}}{\sqrt{n_i}}\right)|0\rangle. \tag{1.25}$$

Energy eigenstate with $E = \hbar\omega N + E_0$ where $N = \sum_{i=1}^d n_i$ is total excitation number. Crucial property

$$[H, \vec{a}^\dagger] = \omega\vec{a}^\dagger. \tag{1.26}$$

1.4 Quantum Mechanics and Relativity

Let us set $\hbar = 1$, $c = 1$ for convenience.[11]

Attempts to set up a relativistic version of quantum mechanics have failed. Let us see why.

[10] No ambiguity for $\vec{p}^{\,2}$ and $\vec{q}^{\,2}$, but useful to consider all second degree polynomials in $\vec{p}$ and $\vec{q}$.

[11] Can be recovered from considerations of physical units.

Non-relativistic and relativistic energy relation

$$e = \frac{\vec{p}^2}{2m}, \qquad \text{vs.} \qquad e^2 = \vec{p}^2 + m^2 \quad \text{or} \quad e = \sqrt{\vec{p}^2 + m^2}. \tag{1.27}$$

Natural guess for relativistic wave equation (Klein–Gordon)

$$\left(-\left(\frac{\partial}{\partial t}\right)^2 + \left(\frac{\partial}{\partial \vec{q}}\right)^2 - m^2 \right) |\psi\rangle = 0. \tag{1.28}$$

Has several conceptual problems:

Probabilistic Properties. The norm $\langle\psi|\psi\rangle$ of non-relativistic QM is conserved only for first-order wave equation.

There is a real conserved quantity

$$Q = \frac{i}{2m} \left(\langle\psi| \frac{\partial}{\partial t} |\psi\rangle - \frac{\partial}{\partial t} \langle\psi|\psi\rangle \right), \tag{1.29}$$

Problem:

- Q is not positive definite.
- Not suitable for probabilistic interpretation![12]

One can define a positive definite measure, but it is not local.

Why consider probabilities in a time slice in the first place?

Causality. Consider the overlap

$$\langle \vec{q}_2 | U(t_2, t_1) | \vec{q}_1 \rangle \tag{1.30}$$

for a pair of spacetime points (t_1, q_1) and (t_2, q_2). Probability amplitude for particle moving from 1 to 2.

Problem:

- Overlap non-zero if points are space-like separated.
- forbidden region: violation of causality?
- at least: exponential suppression (tunnelling).

Negative-Energy Solutions. Second-order wave equation. For every positive-energy solution

$$|\vec{p}, +, t\rangle = \int d^d\vec{q}\, e^{-i\vec{p}\cdot\vec{q} - ie(\vec{p})t} |\vec{q}\rangle \tag{1.31}$$

there is a negative-energy solution

$$|\vec{p}, -, t\rangle = \int d^d\vec{q}\, e^{-i\vec{p}\cdot\vec{q} + ie(\vec{p})t} |\vec{q}\rangle. \tag{1.32}$$

Problems:

[12] As we shall see, Q is rather similar to an electric charge.

- Negative-energy particles not observed.[13]
- Positive-energy particle could fall to negative-energy state. A lot of energy released to produce other particles.

Could insist on positive energies by wave equation

$$i\,\frac{\partial}{\partial t}|\psi\rangle = \sqrt{-\left(\frac{\partial}{\partial\vec{q}}\right)^2 + m^2}\,|\psi\rangle. \tag{1.33}$$

Problems:

- Square root of operator hard to define.
- Certainly non-local wave-equation.

Particle Creation. Special relativity allows energy to be converted to rest mass of particles.

- Relativistic quantum mechanics should allow such processes.
- Quantum mechanics usually assumes a fixed particle number.

Dirac Equation. The Dirac equation was an attempt to overcome some problems

$$\frac{\partial}{\partial t}|\psi\rangle = \alpha^k \frac{\partial}{\partial q^k}|\psi\rangle + \beta m|\psi\rangle. \tag{1.34}$$

Relativistic wave equation; implies Klein–Gordon equation.

Probabilistic interpretation:

- First-order wave equation.
- $\langle\psi|\psi\rangle$ is conserved and positive definite.
- Positivity requires Bose statistics.

Spin:

- Operators α^k imply spin-1/2 particles.
- No spin-0 particles reproducible.
- Half-integer spin requires Fermi statistics.

Negative-energy solutions:

- Exist (with different spin d.o.f.).
- Separation from positive energies is non-local.

Dirac equation has the same problems as Klein–Gordon.

Conclusion. Klein–Gordon and Dirac equations:

- Perfectly acceptable relativistic wave equations.
- No probabilistic interpretation.
- Model without particle production.

[13] Extract energy from making particle faster!

1.5 Conventions

Units. We shall work with natural units $\hbar = c = 1$.

- $c = 299\,792\,458\ \mathrm{m\,s^{-1}}$ therefore $\mathrm{s} := 299\,792\,458\ \mathrm{m}$.
- $\hbar = 1.055\ldots \times 10^{-34}\ \mathrm{kg\,m^2\,s^{-1}}$ therefore $\mathrm{kg} := 2.843\ldots \times 10^{42}\ \mathrm{m^{-1}}$.
- can always reinstall appropriate units by inserting $1 = c = \hbar$.
- particle physics unit electron Volt (eV): $\mathrm{m} = 5.068 \times 10^6\ \mathrm{eV^{-1}}$, $\mathrm{s} = 1.519 \times 10^{15}\ \mathrm{eV^{-1}}$, $\mathrm{kg} = 5.610 \times 10^{35}\ \mathrm{eV}$.
- convert back to SI units: $\mathrm{eV} = 5.068 \times 10^6\ \mathrm{m^{-1}} = 1.519 \times 10^{15}\ \mathrm{s^{-1}} = 1.783 \times 10^{-36}\,\mathrm{kg}$.

Euclidean space. Write a three-vector x as

- x_j with Latin indices $k, l, \cdots = 1, 2, 3$.
- $\vec{x} = (x^1, x^2, x^3) = (x, y, z)$.

Scalar product between two vectors

$$\vec{a}\cdot\vec{b} := \sum_{k=1}^{3} a^k b^k = a^1 b^1 + a^2 b^2 + a^3 b^3. \tag{1.35}$$

Vector square

$$\vec{a}^{\,2} := \vec{a}\cdot\vec{a} = a_1^2 + a_2^2 + a_3^2. \tag{1.36}$$

Totally anti-symmetric epsilon-tensor ε^{ijk} with normalisation

$$\varepsilon^{123} = +1. \tag{1.37}$$

Use to define cross product

$$(a \times b)^k = \varepsilon^{ijk} a^i b^j. \tag{1.38}$$

Minkowski Space. Four vectors, Greek indices $\mu, \nu, \ldots = 0, 1, 2, 3$:

- position vector $x^\mu := (x^0, x^1, x^2, x^3) = (t, \vec{x})$.
- momentum covector $p_\mu := (p_0, p_1, p_2, p_3) = (e, \vec{p})$.

Summation convention: repeated index μ means implicit sum over $\mu = 0, 1, 2, 3$

$$x^\mu p_\mu := \sum_{\mu=0}^{3} x^\mu p_\mu = et + \vec{x}\cdot\vec{p}. \tag{1.39}$$

Minkowski metric: signature $(-{+}{+}{+})$

$$\eta_{\mu\nu} = \eta^{\mu\nu} = \mathrm{diag}(-1, +1, +1, +1). \tag{1.40}$$

Raise and lower indices (wherever needed):

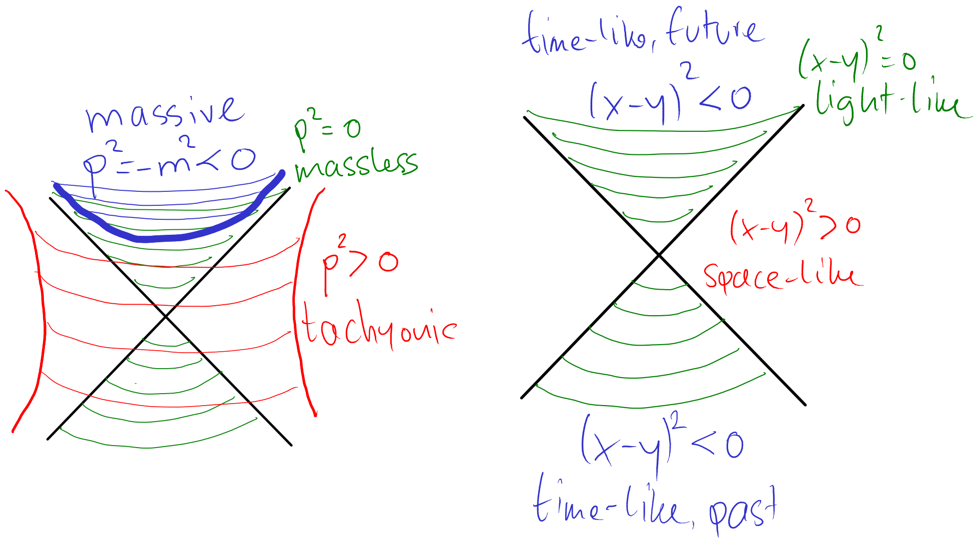
$$x_\mu := \eta_{\mu\nu} x^\mu = (-t, \vec{x}), \qquad p^\mu := \eta^{\mu\nu} p_\mu = (-e, \vec{p}). \tag{1.41}$$

Scalar products of two vectors or two covectors, e.g.

$$p{\cdot}p := -e^2 + \vec{p}^{\,2}. \tag{1.42}$$

Our conventions:

- Mass shell $p^2 = -m^2$: $p^2 < 0$ massive, $p^2 = 0$ massless, $p^2 > 0$ tachyonic.
- Light cone: $(x-y)^2 < 0$ time-like, $(x-y)^2 = 0$ light-like, $(x-y)^2 > 0$ space-like.



(1.43)

Why?

- notation follows space (not time). $\underline{x}^\mu = (t, \underline{\vec{x}})$ $\underline{p}_\mu = (t, \underline{\vec{x}})$
- $x^i = x_i$ but $x^0 = -x_0 = t$.
- $p^i = p_i$ but $p^0 = -p_0 = e$.
- Wick rotations natural: just rotate time $t \to it$ and obtain Euclidean metric.

How to convert?

- flip sign of every $\eta^{\mu\nu}$ and $\eta_{\mu\nu}$.
- find out which (co)vectors match: x^μ and p_μ agree literally, x_μ and p^μ flip the sign.
- flip sign for every scalar product of vectors of same type: e.g. $p^2 + m^2 \leftrightarrow -p^2 + m^2$.
- preserve scalar product between different vectors: $x^\mu p_\mu$.[14]
- note: $\vec{p}$ opposite sign compared to Peskin & Schroeder; mild problem: sign of $\vec{p}$ and e is merely convention.

Name Spaces. We have only 26 Latin letters at our disposal and some are more attractive than others. Have to recycle:

- e may be $2.71\ldots$, but also energy,
- π may be $3.14\ldots$, but also momentum conjugate to field ϕ,
- i may be $\sqrt{-1}$, but also useful for counting.
- κ may look like k or K on the blackboard.

[14] Therefore also $x{\cdot}p$ unchanged (two signs cancel).

- H may be Hamilton function or operator.
- ...

Will typically not say explicitly which letter means what:

- May even use same letter for different meanings in one formula.
- Can guess meaning from the context, e.g. i in $\exp(\pi i \ldots)$ vs. $\sum_{i=1}^{n}$.
- Indices typically do not mix with other symbols.
- Could try to avoid, but may also clutter notation.
- It's a fact of life (and the literature).