A Pedestrian Introduction to the Mathematical Concepts of Quantum Physics[1]

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These notes offer a basic introduction to the primary mathematical concepts of quantum physics, and their physical significance, from the operator and Hilbert space point of view, highlighting more what are essentially the abstract algebraic aspects of quantisation in contrast to more standard treatments of such issues, while also bridging towards the path integral formulation of quantisation. A discussion of the (first) Noether theorem and Lie symmetries is also included to complement the presentation. Emphasis is put throughout, as illustrative examples threading the presentation, on the quantum harmonic oscillator and the dynamics of a charged particle coupled to the electromagnetic field, with the ambition to bring the reader onto the threshold of relativistic quantum field theories with their local gauge invariances as a natural framework for describing relativistic quantum particles in interaction and carrying specific conserved charges.

1 Introduction

1.1 Motivations

With the Summer 2008, the world community of high energy physicists is eagerly awaiting to see the first proton beams circulate in the Large Hadron Collider (LHC), located at the "Centre Européen, Organisation européenne pour la Recherche Nucléaire" (CERN, Geneva, Switzerland; see `http://www.cern.ch`). Using fully electronics equipped detectors filling up huge caverns one hundred meters under ground, at different intersection points of two oppositely moving proton beams in a 27 kilometers long circular collider, these beams being held in their tracks by thousands of over ten meters long superconducting magnets kept cold at 1.9 K by a true liquid helium factory—in itself an engineering feat heretofore never witnessed on the face of this Earth—, teams of thousands of physicists and engineers will start taking data at rates and at energies never before contemplated, to be analysed in search for the few tell-tale signs of discoveries to be made, those expected like those unexpected. Among the primary motivations for this truly encompassing international enterprise bridging peoples from all continents, the hopes are to finally settle some of the crucial questions that our present day theories for the fundamental interactions and the Universe have unearthed and on whose answers so much hinges for any progress forward, and to catch the first glimpses of what must be lying beyond, beyond the known energy and distance and time scales, and thereby reach towards those that prevailed at the origins of time and of our physical Universe.

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	Families			Q
Leptons	ν_e	ν_μ	ν_τ	0
	e^-	μ^-	τ^-	-1
Quarks	u (up)	c (charm)	t (top)	$+\frac{2}{3}$
	d (down)	s (strange)	b (bottom)	$-\frac{1}{3}$

Table 1: The structure of matter: the periodic table of the elementary particles (all of spin $\frac{1}{2}$).

Interaction	Carrier	Spin	Local gauge symmetry
Strong	8 gluons	1	$SU(3)_c$
Electromagnetic	γ (photon)	1	Electroweak interaction
Weak	$W^\pm$, Z_0	1	$SU(2)_L \times U(1)_Y$
Gravity	graviton (?) (spacetime curvature)	2	Spacetime reparametrisations (local Poincaré group ISO(3,1))

Table 2: The structure of the fundamental interactions: from the strongest to the weakest.

One such question is that of the origin of mass, specifically inertial mass of all the known and unknown fundamental constituents of matter and interactions, the elementary particles such as the electron or the quarks (see Tables 1 and 2). Because of its simplicity, and inspired by the dynamics underlying the phenomenon of superconductivity in condensed matter physics with its condensation of electron Cooper pairs, a large consensus favours the so-called Higgs mechanism, in which particles acquire mass, namely inertia, through their interaction energy with a condensate of particles of some other type, the so-called higgs boson. If the higgs boson does indeed exist by Mother Nature's own choice, and not by the theorists' fancies however imaginative and elegant their intellectual inventions may be, it will be discovered at the LHC. When wanting to extend to matter particles the elegance displayed through the so-called gauge symmetries of the fundamental interactions with their specific carriers (see Figure 1), expectations are high for the discovery of a new world prevalent at the higher energies in which each of the known particles of spin 1/2 or 1 is accompanied by a supersymmetric partner of spin 0 or 1/2, respectively. Such new structures lie beyond the limits of the present day accepted model, the so-called Standard Model, having so far survived beyond anyone's best bets the most stringent experimental tests imaginable. More generally, one expects that some form of new physics beyond that Model will start to unravel at the LHC, such as supersymmetry but possibly something we actually never thought of since Mother Nature has this supreme knack for always outwitting us for She seems to never be using the same trick twice. More speculative or fascinating phenomena, as one may like to call them, are also foreseen by some, though based on less solid and more tantalising ideas and conjectures, such as the possibility of "large" extra spatial dimensions having remained hidden to our senses until now, or the production of light black holes if gravity acts at some energy scale in such extra spatial dimensions lower than that at which it appears to be acting in our four dimensional spacetime world. Many more such fascinating features are potential possibilities, all having in common that they would leave behind in LHC data subtle tell-tale signs to be brought to the fore through painstaking analysis, especially through precision studies of the electroweak flavour interactions.

But on which paper music are the scales of the Standard Model and its description of all known fundamental particles and interactions written? By which rules have the harmonies performed by this huge and richly diversified and dynamic symphonic orchestra of the microscopic universe been organised and directed ever since the creation of the physical Universe? Building on the legacy of XIX$^{\text{th}}$ century physics, through the marriage of these two fundamental conceptual revolutions which have been quantum physics, involving as fundamental physical constant $\hbar = h/2\pi$—the reduced Planck constant—, and special relativity, involving as fundamental physical constant c—the speed of light in vacuum as the limiting speed for any actual exchange of energy and momentum, namely any interaction—, physics of the XX$^{\text{th}}$ century

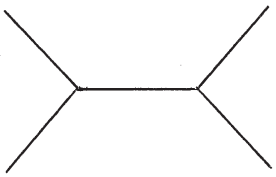


Figure 1: A Feynman diagram: the interaction between two particles through the exchange of the energy and the momentum carried by another particle, the carrier of the interaction.

Quantum $\hbar$ ↘		Special Relativity c ↙ ↘		Gravity G_N ↙
	Relativistic Quantum Field Theory		General Relativity (not quantum)	
Local gauge symmetries	$SU(3)_c \times SU(2)_L \times U(1)_Y$ ↓ ? Grand Unification ↘		Local spacetime diffeomorphisms ↙	
		? Quantum Gravity ?		

Table 3: General conceptual framework: road map to the final unification.

has come to realise that relativistic quantum field theory (QFT), though a conceptual revolution still to be completed in the XXI$^{\text{st}}$ century [1, 2], provides the right harmonies by which to scale up the fundamental dynamics and matter content of our world (see Table 3). A dynamical field possesses both at the same time an oscillatory character and a wavelike spacetime propagation behaviour inclusive of interference properties. As is true for any oscillatory system, when quantised a dynamical field possesses quantum states of quantised energy, the number of these quanta being modified through exchanges of energy, namely interactions through the exchanges of particles. Yet its spacetime dynamics remains wavelike with all its ensuing correlation and interference properties. A quantum field thus achieves the description of a system which at the same time is constituted of particles—when one measures its energy content and its quantum states—and of waves—when one considers its spacetime dynamics and correlations, thereby by-passing any possible issue of conceptual inconsistencies of these dual perceptions of the physical reality.

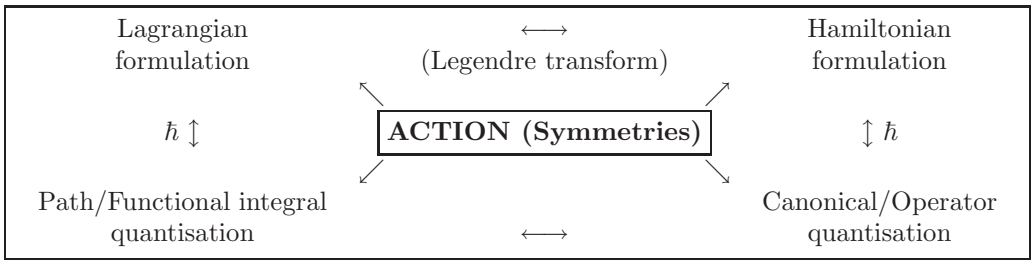
On account of Noether's theorem which associates a conserved dynamical quantity to each generator of a symmetry of a dynamics, relativistic fields evolving within a Minkowski spacetime with its invariance properties under spacetime translations and rotations also possess conserved energy, momentum and angular-momentum. The quantum states of a relativistic quantum field theory thus carry all the hallmarks defining a relativistic quantum particle, namely its energy, momentum—hence relativistic invariant mass m through the relation $E^2 - (\vec{p}c)^2 = (mc^2)^2$, E and $\vec{p}$ being the particle's energy and momentum, respectively—, and also spin. Yet in their spacetime dynamics these particles possess all the properties of waves as well. Furthermore, other conserved quantities that particles may carry, such as the electric charge, are then also associated to some other, non spacetime symmetries, so-called internal symmetries. When these symmetries are realised in such a manner that the effected transformations may be different at each point in spacetime, even though in a continuous fashion throughout spacetime—namely, gauge symmetry transformations—, the result is necessarily the existence of an interaction—a gauge interaction—with its own field of which the quanta are the carrier of that interaction acting between those particles carrying the charge associated to that symmetry. All known fundamental interactions are understood within that framework, given some symmetry group (see Table 3).

The conceptual framework of relativistic quantum field theory—the music paper for the harmonies of the microscopic universe—is thus a most encompassing one producing, through the marriage of $\hbar$ and c, quite a unification of concepts accounting for observational facts of the physical Universe. For instance, note that rather than having to speak and consider all possible particles in the Universe of a given species, say all electrons of the Universe, it suffices to consider the single field filling all of spacetime of which the quanta are that specific particle but existing in different quantum states, hence with different energy-momentum and spin values. All electrons of the Universe are indistinguishable because they are harmonic quantum excitations of a same and single underlying basic physical reality, the electron field. This totally new view point on the reality of the physical world is but one illustration of the unification of concepts unravelled through the construction of quantum field theories as an appropriate framework for the understanding of the fundamental particles and their interactions. Quite a towering achievement of XX$^{\rm th}$ century physics, its fourth but yet unfinished conceptual revolution of the harmonies of the physical Universe!

Indeed, this achievement remains partially unfulfilled since, as is well known, when computing within these theories corrections to quantum processes generated by higher order exchanges of particules, one always encounters divergences generated by fluctuating harmonic modes of the fields at the highest energy or shortest distances scales. However, for all the above gauge theories describing all the fundamental interactions except for gravity, these ultra-violet (UV) divergences may be renormalised away, when expressing all observables in terms of the physical parameters of particles rather than those un-normalised parameters defining the theory before considering its quantised version. Thus even though on a practical level one may live comfortably with such a situation, the fact remains somewhat unsettling, and may well beg for a final theory within which relativistic quantum field theory would find its rightful place in a certain limit, somewhat like Newton's nonrelativistic dynamics is a limiting subcase of Einstein's special relativity dynamics for velocities small compared to c. However, gravity remains an exception in that respect. Even though the third conceptual revolution of XX$^{\rm th}$ century physics, namely General Relativity (GR) resulting from the marriage of c and Newton's constant G_N for the gravitational interaction, has achieved a great unification of concepts in its own right with regards to the Universe at its largest scales where gravity reigns supreme, all attempts so far at a final marriage of all three fundamental constants $\hbar$, c and G_N within the field theory context have failed. Even though GR itself is also a gauge dynamics, though of a different type since the symmetries involved are those of spacetime rather than internal symmetries as is the case for all other three fundamental interactions, the renormalisation programme has not resolved the issue of the UV divergences within a field theory approach to quantum gravity including all of matter and interactions (see Table 2). Thus indeed, the final unification of gravity with the other three fundamental interactions and all forms of matter particles within a single quantum framework remains one of the formidable challenges offered to the young and creative physicists of the XXI$^{\rm st}$ century. XXI$^{\rm st}$ century physics is in search of a next Einstein [1, 2]. Let us all dream and work hard that she will come from Africa!

The purpose of these notes is mainly to provide an introduction, put may be in more mathematical terms and concepts than what is usual, to the basics of quantum physics, whatever the type of dynamical system being considered provided it possesses a classical variational principle description based on an action (see for instance Ref. [3]). This framework encompasses both nonrelativistic as well as relativistic systems, as well as systems with finite or infinite numbers of degrees of freedom, field theories being of course of the latter class. In order to also reach out more to our more mathematically inclined readers, emphasis is laid on the algebraic and geometric aspects of quantisation rather than more traditional trodden paths through the Schrödinger wave equation for instance. Yet, physics illustrations and applications are never far behind, while at the same time aiming towards an understanding of the basics of relativistic quantum field theory, even though the latter as such are not addressed in the present pages. Previous lectures in these Series have already discussed such aspects, with notes available in Refs. [1, 2]. An excellent treatise is Ref. [4]. No attempt shall be made to provide here any further references, and even less an exhaustive list of reviews on these topics. Such material is readily available through references given in those above. In particular, the basics of special relativity are not included either, since many sources for thorough, detailed and clear presentations are easily found as well (for a web site of interest, see `www.phys.unsw.edu.au/einsteinlight/`).

1.2 An outline



As illustrated in the above diagram, the quantity central to our entire discussion is the action of the system. Its dynamical equations of motion follow from it through the variational principle which requires that classical trajectories be extremal points of the action in configuration space. The action also embodies most elegantly the existence of symmetries by being invariant, possibly up to a surface term, under the corresponding transformations of the degrees of freedom of the system. As a consequence, through Noether's theorem, one readily identifies conserved quantities. Because of the necessary requirement of (space)time locality, the action is given by the (space)time integral of a local function of configuration space, namely of the degrees of freedom of the system and their (space)time derivatives. This function is known as the Lagrange function or Lagrangian of the system, or Lagrangian density in the case of fields for which a space and time integration is effected to obtain the action.

One possible path towards quantisation is to directly move from the classical dynamics in its Lagrangian form to the path integral, or functional integral representation of the quantum dynamics (the l.h.s. of the above diagram). Here rather we shall take the "canonical path", namely move from the Lagrangian formulation to the Hamiltonian one for a given system, to which the rules of canonical operator quantisation are then applied to result in a purely abstract algebraic construction defining the quantised system (the r.h.s. of the above diagram). However, we shall show how both realisations of a quantum system are actually equivalent, as much from the mathematical as from the physical point of view. Simply, depending on the problem at hand, one representation may be more convenient than the other to address some issues or computations, while they also speak differently even though in complementary ways to one's physical intuition. The path integral approach has provided much fruitful insight into the nonperturbative dynamics of nonlinear quantum field theories, for instance. Here the operator approach is rather emphasized, first, because it allows to quickly develop a language which mathematicians and physicists alike can easily share, and second, because it is the most straightforward path to grasping why it is that relativistic quantum field theories are in fact theories of relativistic quantum particles, and *vice versa*, simply by relying on the quantum physics of the ordinary one dimensional harmonic oscillator, certainly the simplest of all nontrivial dynamical systems, and in a certain manner thus the "mother" of all quantum field theories, at least in as far as perturbative quantisation and renormalisation of field theories are concerned. This is no small wonder! Indeed, when applied for instance to the electromagnetic interactions of electrons and photons, namely the theory of quantum electrodynamics (QED), such techniques have produced theoretical results precise to eleven decimal places in perfect agreement with experimental results known to the same amazing degree of accuracy. When the art of quantum physics is pushed to such extremes of excellence, any shadow of a discrepancy could be the harbinger for new physics beyond the Standard Model.

It is here that these notes find another of their motivations. Namely, to bring the reader onto the threshold of quantum field theory, a study that he/she could then hopefully embark on afterwards on his/her own, with the help possibly of references such as those in Refs. [1, 2, 4]. One of the ambitions of these notes is to demystify, if necessary, what relativistic quantum field theory actually is in its basic essentials and physical representations, simply as a natural framework for theories of relativistic quantum particles in interaction and characterised by conserved charges in direct correspondence with important symmetries whether of spacetime or internal space geometries.

The outline of the notes is as follows. In the next Section, the Lagrangian formulation of dynamical systems is briefly reviewed. In Section 3, through a Legendre transform, one moves over to the Hamiltonian formulation of the same dynamics, leading to the phase space representation of its degrees of freedom and the ensuing geometrical structures. Section 4 then addresses the canonical quantisation of the Hamiltonian

formulation, emphasizing mostly the purely abstract aspects to that programme, as well as the different representations possible for those abstract structures. It is also at that point that the junction with the path integral quantisation of the classial Lagrangian dynamics is made. Finally, Section 5 discusses the content and consequences of the Noether theorem, a most important result in relation to the existence of continuous (Lie) symmetry groups of transformations leaving the equations of motion of the system invariant and with as further consequence the existence of conservation laws. Some concluding comments are offered in Section 6.

2 Lagrangian Dynamics

2.1 The Action Principle

Let us consider some dynamical system. Its configuration space (the space of all its possible configurations) may be characterised in terms of some manifold M_N of dimension N. For example, in the case of a single point particle moving along an infinite straight line, the possible configurations of the system are any of the positions along that line; its configuration space is thus the real line, $M_N = \mathbb{R}$, a one dimensional space, $N = 1$, for this one degree of freedom system. By extension, the configuration space of a single point particle moving in an N dimensional Euclidean space is $M_N = \mathbb{R}^N$. Likewise, a point particle constrained to be moving on a circle has that circle as configuration space. More generally, constrained to be moving on a sphere of dimension N, its configuration space is the N-sphere, $M_N = S^N$. Such a point particle could also be moving on a torus of dimension N, the cartesian product of N circles, corresponding to a configuration space which is the N dimensional torus, $M_N = T^N$.

The configuration space manifold M_N is also taken to be connected, for if it were to have multiple components, each component could be seen to correspond to a different system, each of these systems being decoupled from one another. Generally, configuration space also comes equipped with some geometry, defined in terms of some metric structure, usually a positive definite one.

Being a manifold, a local system of coordinates may be defined over configuration space, which is also required in order to perform actual calculations and for representing trajectories of the system throughout its configuration space. Generally, such local coordinates are denoted $q^n \in \mathbb{R}$ with $n = 1, 2, \ldots, N$, corresponding to generalised coordinates in configuration space. For example, if configuration space is Euclidean, $M_N = \mathbb{R}^N$, these coordinates could be taken to be cartesian coordinates with respect to some scalar product, or positive definite metric structure defined over configuration space. In the case of the N-sphere, $M_N = S^N$, or the N-torus, $M_N = T^N$, natural coordinates would correspond to some angular parametrisation of the configuration space manifold.

For a realistic system, the number, N, of such degrees of freedom q^n ($n = 1, 2, \ldots, N$) may be extremely large indeed. Imagine a system of N particles moving in three dimensional Euclidean space representing physical space. The associated configuration space is $\mathbb{R}^{3N}$. Choosing to work in terms of cartesian coordinates, these $3N$ degrees of freedom may be expressed as time dependent functions $x^i_\alpha(t)$, with $i = 1, 2, 3$ and $\alpha = 1, 2, \ldots, N$. But in practice for a cubic centimeter of ordinary matter, N is given essentially by Avogadro's number, $N_A \simeq 6 \times 10^{23}$. Note also that the cartesian choice of coordinates may not be the most convenient one for the general N-body system, even already for the $N = 2$ two-body problem for which relative and center-of-mass coordinates are more relevant.

Any time history of the system is associated to some trajectory in configuration space, representing all the successive configurations of the system as it evolves in time. Having specified a local coordinate system over configuration space, such a trajectory is then given by a set of time parametrised functions $q^n(t)$ ($n = 1, 2, \ldots, N$), assumed to be sufficiently smooth for all practical purposes. These functions thus correspond to the degrees of freedom of the system, since they represent the freedom the system has in moving throughout its space of possible configurations as time evolves. Note that the parameter t need not necessarily be the physical time as measured on a clock, even though quite generally t is chosen to be such a physical observable. Indeed t serves the purpose of parametrising the dynamical evolution of the system along its trajectories in configuration space, and any such parametrisation is acceptable. In particular for systems invariant under arbitrary transformations of spacetime coordinates, such as General Relativity, string and M-theory, or even the single parametrised relativistic particle [3], the time evolution parameter t is such an arbitrary choice, of which the physical time itself is then a particular function.

Note that the number N of degrees of freedom need not be finite. The above framework remains applicable for systems with an infinite number of degrees of freedom, including field theories. This number could be infinie countable or even non countable. Consider for instance a real scalar field, $\phi(t,\vec{x}\,) \in \mathbb{R}$, defined over spacetime, $\vec{x}$ parametrising the space dependence of the field. As a matter of fact, that space variable may be seen to correspond to an index, albeit a continuous one, labelling the different degrees of freedom of the system,

$$\phi(t,\vec{x}\,) = \phi^{\vec{x}}(t) \leftrightarrow q^{\vec{x}}(t) \leftrightarrow q^n(t). \tag{1}$$

Even if the label $\vec{x}$ takes values in a continuous set, the number of degrees of freedom is not necessarily infinite non countable. In the case for instance of a torus topology for the spatial directions, through Fourier mode analysis in $\vec{x}$ the number of degrees of freedom is infinite discrete, thus infinite countable with $N \to \infty$. Consequently, at least formally the entire discussion to be developed in these notes extends also to field theories, keeping aware of possible difficulties arising because of an infinite number of degrees of freedom.

Given such a parametrisation of configuration space, how does one determine the dynamics of the system within its configuration space? Through which equations of motion governing its time evolution? As mentioned previously, such dynamics follows from the variational principle applied to a specific quantity known as the action of the system, $S[q^n]$. This action is a **functional** of configuration space, namely a number which is a function of functions, constructed out of the time dependent functions $q^n(t)$ characterising any trajectory of the system in its configuration space. As already indicated, the action is a most encompassing and powerful concept, and plays a central rôle in accounting for the dynamics of the system and all the properties thereof, since,

1. the dynamical equations of motion follow from the action, $S[q^n]$, through the variational principle, and,

2. as will be discussed later on, through Noether's first theorem, invariance of the action under symmetry transformations embodies the existence of conservation laws, namely the existence of conserved quantities for the classical system, corresponding to conserved quantum numbers (such as the electric charge, the spin and angular-momentum, etc.) for the quantised system.

Requiring locality in time, the action must of the form

$$S[q^n] = \int_{t_i}^{t_f} dt\, L(q^n(t), \dot{q}^n(t)), \tag{2}$$

where $L(q^n, \dot{q}^n)$ is some function of the variables q^n and $\dot{q}^n$—viewed at this stage as independent variables with respect to which separate partial derivatives of the function $L(q^n, \dot{q}^n)$ may be taken—, known as the **Lagrange function** or **Lagrangian** of the system. When substituted in the above integral, the Lagrange function is composed with the time dependence $q^n(t)$ representing the flow of the system in time along any specific trajectory in configuration space represented by the functions $q^n(t)$ $(n = 1, 2, \ldots, N)$. In that case, $\dot{q}^n(t)$ then stands for the ordinary derivative of the function $q^n(t)$ with respect to time t, a notation customary in mechanics,

$$\dot{q}^n(t) \equiv \frac{dq^n(t)}{dt} \qquad \text{[generalised velocities]}. \tag{3}$$

The value for the action, $S[q^n]$, is thus associated to a specific trajectory in configuration space corresponding to the time interval $[t_i, t_f]$ for which one has the initial and final configurations $q^n(t_i) = q^n_i$ and $q^n(t_f) = q^n_f$. This trajectory may be pictured as some curved line in configuration space connecting these two end points.

Remarks

1. In the case of a field theory, locality in both time and space implies that the Lagrange function should itself be given as the space integral of a **Lagrangian density**, $\mathcal{L}(\phi, \partial_t\phi, \partial_{\vec{x}}\phi)$, the latter being a local function of the field and its time and spatial derivatives, to be then composed with the time and space dependence of the field, $\phi(t,\vec{x}\,)$, when evaluating the corresponding action,

$$S[\phi] = \int_{t_i}^{t_f} dt \int_{\text{space}} d\vec{x}\, \mathcal{L}(\phi(t,\vec{x}\,), \partial_t \phi(t,\vec{x}\,), \partial_{\vec{x}} \phi(t,\vec{x}\,)), \quad L = \int_{\text{space}} d\vec{x}\, \mathcal{L}(\phi(t,\vec{x}\,), \partial_t \phi(t,\vec{x}\,), \partial_{\vec{x}} \phi(t,\vec{x}\,)). \quad (4)$$

Essentially, the Lagrange function of the system remains given as a sum over the degrees of freedom of the system distinguished by the vector index $\vec{x}$.

2. The Lagrange function may, in general, also have an explicit time dependence, $L(q^n, \dot{q}^n; t)$. However in such a situation, if t stands for the physical time, the energy of the system is not conserved, a situation which does not apply at a fundamental physical level. It is for this reason that at the outset we take the Lagrange function not to have any explicit time dependence, $L(q^n, \dot{q}^n)$. As will be established later on, the Hamiltonian (which coincides with the energy when the time evolution parameter t coincides with the physical time) is then indeed a constant of motion, namely a conserved quantity.

3. One could consider systems for which the Lagrange function may depend on derivatives of the degrees of freedom of order exceeding one, $L(q^n, \dot{q}^n, \ddot{q}^n, \cdots)$. However, through the introduction of an appropriate choice of auxiliary variables of which the equations of motion are such that these extraneous degrees of freedom coincide with the successive time derivatives of the original ones, q^n, it is always possible to bring the description of the system into the above general form, in which the Lagrange function depends on the complete set of degrees of freedom, inclusive of the auxiliary ones, and their first order time derivatives only. Hence no loss of generality is incurred through the above choice of parametrisation for the Lagrange function.

Given the specification of the action functional for the system, its dynamics then follows from the local variational principle, which states that,

> **Variational Principle**: Classical trajectories of the system correspond to local minima (which is possible in the best of cases only, otherwise more generally, they correspond to local extrema or even just stationary points) of the action, $S[q^n]$, of the system.

As shall become clear hereafter, this principle implies differential equations of order two in time, one for each independent degree of freedom $q^n(t)$ of the system, namely specific equations of motion of which the solutions represent the dynamics or time evolution of the classical configurations of the system. Being differential equations of second order in time means also that one must specify for each of these equations of motion two boundary conditions, or integration constants, in order to determine in a unique fashion a specific solution.

The practical implementation of the variational principle proceeds as follows. Imagine that a given (still unknown) classical trajectory $q^n(t)$ determines such a minimum (or stationary point, in general) of the action, and consider then an arbitrary but "infinitesimal" variation $\delta q^n(t)$ in the neighbourhood of $q^n(t)$. The value for the action will thus change accordingly. Expanding the latter to first order in the variation $\delta q^n(t)$, the requirement is that to first order the variation of the action should vanish identically. As we shall see, this latter requirement is to be considered up to surface terms in time, stemming from a contribution to the variation which is a total time derivative. Thus more explicitly and precisely, one has the following representation of the variational principle,

$$\begin{aligned} q^n(t) \quad &\longrightarrow \quad q^n(t) + \delta q^n(t), \quad \delta q^n(t) : \text{ infinitesimal variation}, \\ S[q^n] \quad &\longrightarrow \quad S[q^n + \delta q^n] = S[q^n] + \delta S[q^n] + (\text{higher order terms}), \end{aligned} \quad (5)$$

with

$$\delta S[q^n] = 0, \qquad \text{up to surface terms, or total derivatives.} \quad (6)$$

As mentioned above, the latter requirement translates into a set of differential equations of motion for the functions $q^n(t)$, the Euler–Lagrange equations of motion.

2.2 The Euler–Lagrange equations of motion

Let us proceed with the explicit evaluation of $\delta S[q^n]$ to first order in $\delta q^n(t)$,

$$\begin{aligned}
\delta S[q^n] &= S[q^n + \delta q^n] - S[q^n] && \text{[only to first order in } \delta q^n\text{]} \\
&= \int_{t_i}^{t_f} dt\, \{L(q^n + \delta q^n, \dot{q}^n + \delta \dot{q}^n) - L(q^n, \dot{q}^n)\} && \left[\delta \dot{q}^n(t) = \frac{d}{dt}\delta q^n(t)\right] \\
&= \int_{t_i}^{t_f} dt \left\{ \delta q^n \frac{\partial L}{\partial q^n} + \frac{d}{dt}\delta q^n \frac{\partial L}{\partial \dot{q}^n} \right\} \\
&= \int_{t_i}^{t_f} dt\, \delta q^n \left[\frac{\partial L}{\partial q^n} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^n} \right] + \int_{t_i}^{t_f} dt \frac{d}{dt}\left[\delta q^n \frac{\partial L}{\partial \dot{q}^n} \right], \qquad (7)
\end{aligned}$$

where in the last line an integration by parts was effected in order to isolate all terms in δq^n as factorised contributions. In (7), the first term is given as an integral over the entire "volume" of the time interval $[t_i, t_f]$ (in the case of field theory, it is given as an integral also over the volume of space), hence that term is the "volume" term contribution to $\delta S[q^n]$. On the other hand, the second contribution in (7) is a surface term in time, being given by the time integration of the total time derivative of the specific combination $\delta q^n \partial L/\partial \dot{q}^n$, of which the value thus depends only on the values of $q^n(t)$, $\dot{q}^n(t)$ and $\delta q^n(t)$ at t_i and t_f, namely the boundary or "surface" of the time interval $[t_i, t_f]$ (again in the case of field theory, one then gets genuine surface terms of space and time). Hence that second contribution is the "surface" term contribution to $\delta S[q^n]$.

Another remark is worth to be made explicit here. In the above expressions, the so-called Einstein convention for summation is used. Namely whenever an identical index n appears in two quantities that are multiplied with one another, a summation over $n = 1, 2, \ldots, N$ is implicit. For instance

$$\delta q^n \frac{\partial L}{\partial q^n} \equiv \sum_{n=1}^{N} \delta q^n \frac{\partial L}{\partial q^n}. \qquad (8)$$

This notation is very common and most widely used in the physics literature. The same practice is thus followed throughout these notes, unless otherwise specified.

Since according to the variational principle the condition $\delta S[q^n] = 0$ (up to the surface term contributions) is to be met whatever the variations $\delta q^n(t)$, a vanishing "volume" contribution is guaranteed only provided the following equations are obeyed for each of the degrees of freedom q^n,

$$\frac{d}{dt}\frac{\partial L(q^n(t), \dot{q}^n(t))}{\partial \dot{q}^n} - \frac{\partial L(q^n(t), \dot{q}^n(t))}{\partial q^n} = 0, \qquad \text{for all } n = 1, 2, \ldots, N. \qquad (9)$$

Even though discussed explicitly hereafter, it should already be clear that these equations are in general second order differential equations in time for the functions $q^n(t)$, of which the solutions thus determine the possible classical trajectories in configuration space, depending on a specific choice of boundary conditions. These equations are the **Euler–Lagrange equations of motion** of the system.

The specification of boundary conditions may or may not be done according to whether one wishes also the "surface" term contribution in (7) to vanish identically or not. For instance, keeping the end values $q_i^n = q^n(t_i)$ and $q_f^n = q^n(t_f)$ fixed for the time interval $[t_i, t_f]$ amounts to considering arbitrary variations $\delta q^n(t)$ which are necessarily such that

$$\delta q^n(t_i) = 0, \quad \delta q^n(t_f) = 0. \qquad (10)$$

In other words, requiring the variational principle in a "strong" sense, meaning that $\delta S[q^n]$ ought to vanish including the "surface" contribution, imposes as boundary conditions in order to solve the Euler–Lagrange equations of motion the following integration constants

$$q^n(t_i) = q_i^n, \quad q^n(t_f) = q_f^n. \qquad (11)$$

However quite often such a choice is not convenient, or does not correspond to the actual physical situation being considered. This is the case for instance when both the initial configuration and generalised velocity

of the system are specified, $q^n(t_i) = q_i^n$ and $\dot{q}^n(t_i) = \dot{q}_i^n$, and under such a circumstance the "surface" contribution to $\delta S[q^n]$ generally does not vanish. Consequently, it is usually preferable to impose the variational principle in a "weak" sense, meaning that only the "volume" contribution to $\delta S[q^n]$ is required to vanish, as was discussed above. Imposing the variational principle in a strong sense by also requiring the "surface" term to vanish is very often too restrictive.

Comments

1. It may readily be established that two Lagrange functions for a same configuration space q^n which differ by a total time derivative of an arbitrary function $F(q^n)$ of the configuration space coordinates in fact lead to identical Euler–Lagrange equations of motion, hence describe identical dynamics in that configuration space,

$$L'(q^n, \dot{q}^n) = L(q^n, \dot{q}^n) + \frac{dF(q^n)}{dt} = L(q^n, \dot{q}^n) + \dot{q}^n \frac{\partial F(q^n)}{\partial q^n}. \tag{12}$$

This result follows by considering the difference of the Euler–Lagrange equations associated to the two Lagrange functions, and establishing that this difference vanishes identically irrespective of the choice for $F(q^n)$ (in the context of the exterior differential calculus on the configuration space manifold, the calculation is equivalent to showing that the squared exterior derivative vanishes identically). But a more immediate proof notices that the additional term $dF(q^n)/dt$ simply induces an additional surface term contribution to the action $S[q^n]$. Since the Euler–Lagrange equations follow from a volume contribution only, such a surface term contribution simply cannot affect these equations of motion. This result also shows that when the dynamics of a system follows from the variational principle, the associated action is at best defined up to such total derivative contributions.

The fact that the Euler–Lagrange equations of motion are left invariant under such a change in action implies only that the **classical** dynamics is independent of such redefinitions of the action. However, this is not necessarily the case at the quantum level. Indeed, when configuration space possesses nontrivial topology, in particular non contractible cycles (in other words, when the first homotopy group or fundamental group of the configuration space is nontrivial), this arbitrariness in the choice of Lagrange function carries some physical and in principle observable consequences, often leading to extra parameters of a purely quantum character of which the value must be quantised.

The issue of the inverse variational problem, namely the determination of a Lagrange function given a set of equations of motion, is also an interesting one, but is not discussed here. Let us only say that generically, the choice is unique modulo the arbitrariness discussed above, even though there exist large classes of exceptions for which even an infinite number of different actions all lead to identical equations of motion.

2. Let us now make more explicit the expression for the Euler–Lagrange equations of motion (9),

$$\frac{\partial^2 L}{\partial \dot{q}^{n_1} \partial \dot{q}^{n_2}} \, \ddot{q}^{n_2} \; + \; \frac{\partial^2 L}{\partial \dot{q}^{n_1} \partial q^{n_2}} \, \dot{q}^{n_2} \; - \; \frac{\partial L}{\partial q^{n_1}} = 0. \tag{13}$$

In this collection of equations, one for each $n = 1, 2, \ldots, N$, the terms multiplying the generalised accelerations $\ddot{q}^{n_2}$ define, at each point in the velocity phase space $(q^n, \dot{q}^n)$, a $N \times N$ square matrix known as the Hessian of the Lagrange function,

$$H_{n_1 n_2}(q^n, \dot{q}^n) = \frac{\partial^2 L(q^n, \dot{q}^n)}{\partial \dot{q}^{n_1} \partial \dot{q}^{n_2}}. \tag{14}$$

Thus depending on whether this matrix is regular or not, these equations may or may not be used to express all accelerations in terms of the generalised positions and velocities, in the form

$$\ddot{q}^n(t) = g^n(q^n(t), \dot{q}^n(t)), \tag{15}$$

for some functions $g^n(q^n, \dot{q}^n)$. Clearly in such a situation, one recovers equations of motion of the Newton type, $m\ddot{\vec{r}}(t) = \vec{F}(\vec{r}(t), \dot{\vec{r}}(t))$, which are second order in time derivatives for each of the degrees of freedom. Thus a system for which the Lagrange function has a regular Hessian,

$$\det \frac{\partial^2 L}{\partial \dot{q}^{n_1} \partial \dot{q}^{n_2}} \neq 0, \tag{16}$$

is said to be a **regular** system (strictly speaking, it is the Lagrangian used to described the dynamics of that system which is regular).

In contradistinction, a **singular** system is one for which the Hessian is singular,

$$\det \frac{\partial^2 L}{\partial \dot{q}^{n_1} \partial \dot{q}^{n_2}} = 0. \tag{17}$$

Consequently, the Hessian then possesses at least one eigenvector of vanishing eigenvalue. Denoting such zero eigenvectors by $V^n_\alpha(q^n, \dot{q}^n)$ with the label α distinguishing all such independent zero eigenvectors, and projecting the Euler–Lagrange equations onto any one of these eigenvectors, one obtains a series of constraints for the coordinates q^n and their velocities $\dot{q}^n$,

$$V^{n_1}_\alpha(q^n, \dot{q}^n) \left[\frac{\partial^2 L(q^n, \dot{q}^n)}{\partial \dot{q}^{n_1} \partial q^{n_2}} \dot{q}^{n_2} - \frac{\partial L(q^n, \dot{q}^n)}{\partial q^{n_1}} \right] = 0. \tag{18}$$

Hence singular systems are constrained systems. An important class of constrained systems is that of gauge invariant systems, of which General Relativity, Yang-Mills theories or string theories are famous and most relevant and interesting examples.

3. At the classical level, the absolute (numerical) and physical (physical dimension) normalisation of the action or Lagrange function are totally irrelevant. Rescaling these quantities by a dimensional or dimensionless factor does not affect the Euler–Lagrange equations of motion which are homogeneous (of weight one) in the Lagrange function. However when it comes to quantum mechanics, this is no longer irrelevant and as a matter of fact it is essential that the physical dimension of the action be that of Planck's (reduced) constant $\hbar = h/2\pi$. Likewise, rescaling the absolute normalisation of the action by a dimensionless factor also has physical consequences or significance. Furthermore, in order that the quantum dynamics be unitary and thus preserves quantum probabilities, it is a sufficient condition that the action be a real quantity under complex conjugation, even in the presence of complex valued degrees of freedom.

2.3 Illustrative examples

2.3.1 Newton's mechanics of conservative systems

Consider a system of N nonrelativistic massive particles of masses m_α, $\alpha = 1, 2, \ldots, N$, and of position vectors $\vec{r}_\alpha(t)$ with respect to some choice of inertial frame (these position vectors may be decomposed in terms of their cartesian coordinates, since space is taken to be Euclidean in Newton's mechanics). These particles are subjected to a collection of forces which are all conservative (which means that those forces that may not necessarily be conservative develop anyway an identically vanishing power or work, hence do not contribute to the energy balance of the system; a typical example is that of a force perpendicular at all times to the velocity $\dot{\vec{r}}(t)$). Consequently, these forces may be characterised by their total potential energy $V(\vec{r}_\alpha)$.

Furthermore, each of the particles possesses a kinetic energy associated to its velocity, leading to the total kinetic energy of the system,

$$T(\dot{\vec{r}}_\alpha) = \sum_{\alpha=1}^{N} \frac{1}{2} m_\alpha \, \dot{\vec{r}}_\alpha{}^2. \tag{19}$$

In order to reproduce Newton's equations of motion for this system as Euler–Lagrange equations of motion for some choice of Lagrange function, let us consider the following combination of T and V,

$$L(\vec{r}_\alpha, \dot{\vec{r}}_\alpha) = T(\dot{\vec{r}}_\alpha) \, - \, V(\vec{r}_\alpha) = \sum_{\alpha=1}^{N} \frac{1}{2} m_\alpha \dot{\vec{r}}_\alpha{}^2 \, - \, V(\vec{r}_\alpha). \tag{20}$$

To establish the Euler–Lagrange equations of motion for this choice of Lagrange function, one needs to consider the partial derivatives of L separately with respect to each of the cartesian coordinates of either

$\vec{r}_\alpha$ or $\dot{\vec{r}}_\alpha$. For a given particle, namely value of α, these quantities combine into a vector quantity again, of which the cartesian components are these partial derivatives. Hence the compact notation used hereafter for such partial derivatives, in which a partial derivative with respect to a vector stands for the vector of which the components are the successive partial derivatives with respect to the components of the vector with respect to which the vector partial derivative is taken. Therefore, one obtains

$$\frac{\partial L}{\partial \vec{r}_\alpha} = -\frac{\partial V}{\partial \vec{r}_\alpha}, \quad \frac{\partial L}{\partial \dot{\vec{r}}_\alpha} = m_\alpha \dot{\vec{r}}_\alpha, \tag{21}$$

leading to the Euler–Lagrange equations of motion

$$m_\alpha \ddot{\vec{r}}_\alpha(t) = -\frac{\partial V(\vec{r}_\alpha(t))}{\partial \vec{r}_\alpha} = \vec{F}_\alpha(\vec{r}_\alpha(t)). \tag{22}$$

These are indeed precisely Newton's equations of motion for the system.

Note that by taking the scalar product of the equation of motion for the particle α with its velocity $\dot{\vec{r}}_\alpha$, and then summing over all particles, any solution $\vec{r}_\alpha(t)$ to the equations of motion obeys the following identity,

$$\sum_{\alpha=1}^{N} \dot{\vec{r}}_\alpha \cdot \left(m_\alpha \ddot{\vec{r}}_\alpha \right) = \sum_{\alpha=1}^{N} \dot{\vec{r}}_\alpha \cdot \vec{F}_\alpha = -\sum_{\alpha=1}^{N} \dot{\vec{r}}_\alpha \cdot \frac{\partial V}{\partial \vec{r}_\alpha}. \tag{23}$$

However since on both sides of this identity one recognises total time derivatives, it may also be expressed as,

$$\frac{d}{dt}\left[\sum_{\alpha=1}^{N} \frac{1}{2} m_\alpha \dot{\vec{r}}_\alpha{}^2 + V(\vec{r}_\alpha) \right] = 0, \tag{24}$$

namely

$$\frac{d}{dt}\left[T + V \right] = 0. \tag{25}$$

In other words, the quantity

$$E = T + V, \tag{26}$$

which defines the total mechanical energy of the system is a constant of motion. This means that the value it takes for a given solution to the equations of motion is time independent, a constant in time, even though the specific value that is obtained varies from one solution to another since it depends for example on the initial values for both the positions, $\vec{r}_\alpha$, and velocities, $\dot{\vec{r}}_\alpha$. Later on, we shall understand on the basis of Noether's (first) theorem that the existence of a such a conserved energy is consequence of a symmetry of the system, namely its invariance under arbitrary constant translations in time.

2.3.2 The free nonrelativistic particle

According to the previous general discussion, the Lagrange function for a single nonrelativistic massive particle free of the action of any forces is simply

$$L = \frac{1}{2} m \dot{\vec{r}}^{\,2}. \tag{27}$$

It thus follows that the equation of motion is

$$m \ddot{\vec{r}}(t) = \vec{0}. \tag{28}$$

Specifying as boundary conditions for these second order differential equations the initial values

$$\vec{r}_0 = \vec{r}(t_0), \qquad \vec{v}_0 = \dot{\vec{r}}(t_0), \tag{29}$$

the solution reads

$$\vec{r}(t) = \vec{r}_0 + \vec{v}_0\,(t - t_0), \qquad \dot{\vec{r}}(t) = \vec{v}_0, \tag{30}$$

representing a straight line trajectory at a constant velocity. Hence not only is the total energy of the particle a constant of motion,

$$E = T = \frac{1}{2} m \dot{\vec{r}}^{\,2} = \frac{1}{2} m \vec{v}_0^{\,2}, \tag{31}$$

but so is its linear or velocity **momentum**,

$$\vec{p}(t) = m \dot{\vec{r}}(t) = m \vec{v}_0. \tag{32}$$

Furthermore its **angular-momentum**,

$$\vec{L}(t) = \vec{r}(t) \times \vec{p}(t) = m \vec{r}(t) \times \dot{\vec{r}}(t) = m \vec{r}_0 \times \vec{v}_0, \tag{33}$$

is then also a constant of motion. In the same manner as for the energy, we shall understand later on how conservation of momentum is related to invariance of the system under constant translations in space, and conservation of angular-momentum to invariance under constant rotations in space.

2.3.3 The nonrelativistic one dimensional harmonic oscillator

Consider a spring of spring constant k allowed to be deformed along a single cartesian direction, with a mass m attached at one of its ends, the other being kept fixed. Denoting the elongation of the spring by x ($x = 0$ being the value for x when the spring in its natural undeformed state, while $x < 0$ corresponds to a contracted state of the spring), the force developed by the spring is

$$F(x) = -kx, \qquad F(x) = -kx = -\frac{dV(x)}{dx}, \tag{34}$$

with potential energy

$$V(x) = \frac{1}{2} k x^2. \tag{35}$$

Consequently the Lagrange function for this system is simply

$$L(x, \dot{x}) = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2, \tag{36}$$

with as equation of motion

$$m \ddot{x}(t) = -kx(t). \tag{37}$$

Defining the quantity

$$\omega = \sqrt{\frac{k}{m}} > 0, \tag{38}$$

one thus obtains the simple linear harmonic equation

$$\ddot{x}(t) \, + \, \omega^2 \, x(t) = 0. \tag{39}$$

Being a linear differential equation of order two, its general solution is the superposition of any two linearly independent elements in the set of its solutions. Taking for the latter $\cos \omega(t - t_0)$ and $\sin \omega(t - t_0)$, where t_0 is some time at which the following initial values are specified as boundary conditions,

$$x(t_0) = x_0, \quad \dot{x}(t_0) = v_0, \tag{40}$$

it readily follows that the solution is given as

$$x(t) = x_0 \cos \omega(t - t_0) + \frac{v_0}{\omega} \sin \omega(t - t_0), \quad \dot{x}(t) = v_0 \cos \omega(t - t_0) - \omega x_0 \sin \omega(t - t_0), \tag{41}$$

or equivalently

$$x(t) = C \cos \left[\omega(t - t_0) - \varphi_0 \right], \quad \dot{x}(t) = -C\omega \sin \left[\omega(t - t_0) - \varphi_0 \right], \tag{42}$$

with

$$C = \sqrt{x_0^2 + \frac{v_0^2}{\omega^2}}, \qquad \cos \varphi_0 = \frac{x_0}{C}, \qquad \sin \varphi_0 = \frac{v_0/\omega}{C}, \qquad \tan \varphi_0 = \frac{v_0/\omega}{x_0}. \tag{43}$$

The latter form makes explicit that the solution is periodic with period $T = 2\pi/\omega = 2\pi\sqrt{m/k}$, and purely harmonic since only the mode with the frequency $\nu = \omega/2\pi$ is involved, ω thus being its angular frequency.

Because of the acting force of the spring the momentum of the particle is not conserved. However its energy is and takes the value

$$E = \frac{1}{2}m\dot{x}^2(t) + \frac{1}{2}kx^2(t) = \frac{1}{2}mv_0^2 + \frac{1}{2}kx_0^2. \tag{44}$$

Alternative representations of the general solution are of course possible. One which will become of relevance when quantising the system is obtained by using as generating basis of the solutions the pure imaginary exponentials, namely

$$x(t) = \frac{1}{\sqrt{2m\omega}}\left[\,\alpha_0\, e^{-i\omega(t-t_0)} \,+\, \alpha_0^*\, e^{i\omega(t-t_0)}\,\right]. \tag{45}$$

Here, the normalisation is chosen for later convenience, while α_0 stands for a complex valued integration constant. That the second contribution in this sum involves the complex conjugate coefficient α_0^* follows from the requirement that the solution $x(t)$ be real under complex conjugation. Hence the two real boundary conditions necessary to uniquely specify a solution to the equation of motion are traded for a single complex valued boundary condition. Of course, the value for α_0 may be expressed in terms of a different choice of integration constants, such as for instance the one made above in terms of x_0 and v_0. One finds in that case,

$$\alpha_0 = \sqrt{\frac{m\omega}{2}}\left[x_0 + \frac{i}{\omega}v_0\right], \qquad \alpha_0^* = \sqrt{\frac{m\omega}{2}}\left[x_0 - \frac{i}{\omega}v_0\right]. \tag{46}$$

More generally, defining

$$\alpha(t) = \alpha_0\, e^{-i\omega(t-t_0)}, \qquad \alpha^*(t) = \alpha_0^*\, e^{i\omega(t-t_0)}, \tag{47}$$

one has

$$x(t) = \frac{1}{\sqrt{2m\omega}}\,[\,\alpha(t) \,+\, \alpha^*(t)\,], \qquad p(t) = m\dot{x}(t) = -\frac{im\omega}{\sqrt{2m\omega}}\,[\,\alpha(t) \,-\, \alpha^*(t)\,], \tag{48}$$

and conversely

$$\alpha(t) = \sqrt{\frac{m\omega}{2}}\left[x(t) + \frac{i}{m\omega}p(t)\right], \qquad \alpha^*(t) = \sqrt{\frac{m\omega}{2}}\left[x(t) - \frac{i}{m\omega}p(t)\right]. \tag{49}$$

These expressions will become of relevance when considering the Hamiltonian formulation of this system, and subsequently its canonical quantisation.

2.3.4 The simple pendulum

As an example of a coordinate which is not cartesian, let us turn now to the simple pendulum. Namely a string of inextensible length ℓ fixed at one end and with a point mass m attached at the other, free to oscillate in a fixed vertical plane and being kept straight because of its inner tension. The motion of the mass m is thus circular and of radius ℓ, requiring a single degree of freedom to specify its configuration at any instant in time, for which we shall take the angular position $\theta(t)$ of the mass m measured with respect to the downward vertical direction. Ignoring any possible friction, the mass m is subjected to only two forces. One of these is the force of gravity or weight, $m\vec{g}$, of the mass m, a conservative force of potential energy $V(\theta) = mg\ell(1 - \cos\theta)$. The other is the tension $T(t)$ in the string, but being perpendicular at all times to the velocity of the particle, it does not develop any work nor power and is thus irrelevant as far as the balance of energy of the system is concerned.

Knowing, on basis of the kinematics of the system, that the norm of the velocity of the mass is $\ell|\dot{\theta}(t)|$, it follows from our previous discussion that the Lagrange function for this system is simply

$$L(\theta, \dot{\theta}) = \frac{1}{2}m\ell^2\dot{\theta}^2 - mg\ell(1 - \cos\theta). \tag{50}$$

Consequently

$$\frac{\partial L}{\partial \theta} = -mg\ell \sin\theta, \qquad \frac{\partial L}{\partial \dot{\theta}} = m\ell^2 \dot{\theta}, \tag{51}$$

so that the Euler–Lagrange equation of motion of the pendulum is

$$\ddot{\theta}(t) + \frac{g}{\ell} \sin\theta(t) = 0, \tag{52}$$

a nonlinear differential equation of order two at the basis of the construction of Jacobi's elliptic functions. This is indeed also the equation which follows from Newton's equation of motion for this system. From the latter equation, one may also establish the value for the tension $T(t)$ in the string,

$$T(t) = mg\left[\frac{\ell}{g}\dot{\theta}^2(t) + \cos\theta(t)\right]. \tag{53}$$

In the limit of small oscillations, such that $\theta \ll 1$ radian, by linearisation with $\sin\theta \simeq \theta + \cdots$ and $\cos\theta \simeq 1 - \theta^2/2 + \cdots$, the Lagrange function and equation of motion become

$$L \simeq \frac{1}{2}m\left(\ell\dot{\theta}\right)^2 - \frac{1}{2}m\left(\frac{g}{\ell}\right)(\ell\theta)^2, \tag{54}$$

$$\ddot{\theta} + \frac{g}{\ell}\theta = 0. \tag{55}$$

These expressions are recognised to be equivalent to those for a harmonic oscillator of degree of freedom $(\ell\theta)$ and angular frequency

$$\omega = \sqrt{\frac{g}{\ell}}. \tag{56}$$

Hence the period of a simple pendulum in the limit of small oscillations is

$$T = 2\pi\sqrt{\frac{\ell}{g}}. \tag{57}$$

It is by observing and then measuring such a period of a chandelier in a church in Pisa where he attended Mass, that Galilei Galileo started thinking about mechanics... The rest is history.

2.3.5 The charged particle in a background electromagnetic field

Let us consider a nonrelativistic particle of mass m and position vector $\vec{r}(t)$ (with respect to some inertial frame), subjected to conservative forces of which the total potential energy is denoted $V(\vec{r})$. In addition, the particle possesses a charge q, and is subjected to a background electromagnetic field, of electric field $\vec{E}(t,\vec{r})$ and magnetic field $\vec{B}(t,\vec{r})$. Associated to these fields one has the scalar and vector electromagnetic potentials $\Phi(t,\vec{r})$ and $\vec{A}(t,\vec{r})$, respectively. One of the purposes of the present illustration is to recover the relation existing between these potentials and the electric and magnetic fields. This will be done by deriving the equations of motion given a Lagrange function, and identifying these equations with the Lorentz force developed by the electric and magnetic fields.

In that spirit, let us consider the following Lagrange function,

$$L(\vec{r},\dot{\vec{r}};t) = \frac{1}{2}m\dot{\vec{r}}^2 - q\Phi(t,\vec{r}) + q\dot{\vec{r}}\cdot\vec{A}(t,\vec{r}) - V(\vec{r}). \tag{58}$$

Except perhaps for the term involving the vector potential $\vec{A}(t,\vec{r})$, this Lagrange function is recognised once again to be of the form $T-V$, with T the nonrelativistic kinetic energy of the particle, and V standing for the total potential energy comprised, in the present case, of the potential energy $V(\vec{r})$ as well as the term $q\Phi(t,\vec{r})$. Indeed, in the static case, it is well known that the scalar electromagnetic potential $\Phi(\vec{r})$ is related to the electric field by $\vec{E}(\vec{r}) = -\vec{\nabla}\Phi(\vec{r})$, while the potential energy of a charge q in such a field is $q\Phi(\vec{r})$. Even for a time dependent electromagnetic scalar potential, we have kept this contribution in the Lagrange function. Note also that we have here an example of a Lagrange function which carries an

explicit time dependence when the background fields $\Phi(t,\vec{r}\,)$ and $\vec{A}(t,\vec{r}\,)$ vary in time, which is certainly the case when the electromagnetic fields $\vec{E}(t,\vec{r}\,)$ and $\vec{B}(t,\vec{r}\,)$ vary in time. An example is that of a passing electromagnetic wave acting on the charged particle.

Since we are to take partial variations with respect to the components of the position and velocity vectors, $\vec{r}$ and $\dot{\vec{r}}$, let us now make these contributions explicit in the expression of the Lagrange function, and denote the associated cartesian components as x^i and $\dot{x}^i$, with $i = 1, 2, 3$, while the index i may be freely raised or lowered (since the metric is Euclidean, given by δ_{ij}). Then

$$L(x^i, \dot{x}^i; t) = \frac{1}{2} m (\dot{x}^i)^2 - q\Phi(t, x^i) + q\dot{x}^i\, A_i(t, x^i) - V(x^i). \tag{59}$$

Once again, here it is understood that the implicit summations over repeated indices in a product are to be summed over all their values, $i = 1, 2, 3$ (hence this also applies to the term in $(\dot{x}^i)^2$).

One then readily has

$$\frac{\partial L(x^i, \dot{x}^i; t)}{\partial x^i} = -q \frac{\partial \Phi(t, x^i)}{\partial x^i} + q\dot{x}^j \frac{\partial A_j(t, x^i)}{\partial x^i} - \frac{\partial V(x^i)}{\partial x^i}, \tag{60}$$

$$\frac{\partial L(x^i, \dot{x}^i; t)}{\partial \dot{x}^i} = m\dot{x}_i + qA_i(t, x^i), \tag{61}$$

hence

$$\frac{d}{dt} \frac{\partial L(x^i, \dot{x}^i; t)}{\partial \dot{x}^i} = m\ddot{x}_i + q\dot{x}^j \frac{\partial A_i(t, x^i)}{\partial x^j} + q \frac{\partial A_i(t, x^i)}{\partial t}. \tag{62}$$

Consequently, the Euler–Lagrange equations of motion become,

$$m\ddot{x}_i(t) = -q \frac{\partial \Phi(t, x^i(t))}{\partial x^i} - q \frac{\partial A_i(t, x^i(t))}{\partial t} + q\dot{x}^j(t) \left[\frac{\partial A_j(t, x^i(t))}{\partial x^i} - \frac{\partial A_i(t, x^i(t))}{\partial x^j} \right] - \frac{\partial V(x^i(t))}{\partial x^i}. \tag{63}$$

The term in the gradient of the potential energy $V(x^i)$ is of course identified with the (sum of the) mechanical force(s) to which the particle is subjected,

$$F_i(x^i) = -\frac{\partial V(x^i)}{\partial x^i}, \qquad \vec{F}(\vec{r}\,) = -\vec{\nabla} V(\vec{r}\,). \tag{64}$$

The remaining contributions in the r.h.s. of the above equations of motion should thus be identifiable with the Lorentz force,

$$\vec{F}_{\text{Lorentz}}(\vec{r}, \dot{\vec{r}}; t) = q\vec{E}(t, \vec{r}\,) + q\dot{\vec{r}} \times \vec{B}(t, \vec{r}\,). \tag{65}$$

Consequently, the electric field is to be defined according to

$$E_i(t, x^i) = -\frac{\partial \Phi(t, x^i)}{\partial x^i} - \frac{\partial A_i(t, x^i)}{\partial t}, \quad \vec{E}(t, \vec{r}\,) = -\vec{\nabla}\Phi(t, \vec{r}\,) - \frac{\partial \vec{A}(t, \vec{r}\,)}{\partial t}. \tag{66}$$

For what concerns the magnetic field, let us set

$$\vec{B}(t, \vec{r}\,) = \vec{\nabla} \times \vec{A}(t, \vec{r}\,), \quad B_i(t, x^i) = \epsilon^{ijk} \frac{\partial A_k(t, x^i)}{\partial x^j}, \tag{67}$$

ϵ^{ijk} being the totally antisymmetry invariant tensor in three dimensional Euclidean space, with the value $\epsilon^{123} = +1$. Conversely, one then has

$$\frac{\partial A_j(t, x^i)}{\partial x^i} - \frac{\partial A_i(t, x^i)}{\partial x^j} = \epsilon^{ijk}\, B_k. \tag{68}$$

Consequently, the contributions in $\dot{x}^i$ to the equations of motion are identified as

$$\dot{x}^j \left[\frac{\partial A_j(t, x^i)}{\partial x^i} - \frac{\partial A_i(t, x^i)}{\partial x^j} \right] = \dot{x}^j \epsilon^{ijk} B_k(t, x^i) = \left(\dot{\vec{r}} \times \vec{B}(t, \vec{r}\,) \right)^i. \tag{69}$$

In conclusion, combining all the contributions and writing the equations in vector form again, we have finally obtained for the vector equation of motion of the particle

$$m\ddot{\vec{r}}(t) = q\vec{E}(t,\vec{r}(t)) + q\dot{\vec{r}}(t) \times \vec{B}(t,\vec{r}(t)) + \vec{F}(\vec{r}(t)), \tag{70}$$

where the electric and magnetic fields making up the electromagnetic field are related to the scalar and vector electromagnetic potentials by,

$$\vec{E}(t,\vec{r}) = -\vec{\nabla}\Phi(t,\vec{r}) - \frac{\partial \vec{A}(t,\vec{r})}{\partial t}, \qquad \vec{B}(t,\vec{r}) = \vec{\nabla} \times \vec{A}(t,\vec{r}). \tag{71}$$

This analysis has thus established that the Lagrange function (58) indeed describes the dynamics of a nonrelativistic charged massive particle subjected to a background electromagnetic field, as well as some mechanical conservative forces. But additionally, we have identified the relations between the electromagnetic field, namely its electric and magnetic components $\vec{E}$ and $\vec{B}$, with the associated scalar and vector components, Φ and $\vec{A}$, of the electromagnetic potential. Note that the Lagrange function is given in terms of the latter and not the electric and magnetic fields. The reasons for this feature are far reaching and physically most significant, but are not discussed here.

Let us also take the opportunity to discuss here different aspects related to these electromagnetic potential components. Given the fundamental identities of vector analysis,

$$\vec{\nabla} \cdot (\vec{\nabla} \times \vec{V}(\vec{r})) = 0, \qquad \vec{\nabla} \times \vec{\nabla} S(\vec{r}) = \vec{0}, \tag{72}$$

valid for any vector, $\vec{V}(\vec{r})$, and scalar, $S(\vec{r})$, fields, it follows that given the relations in (71) one has for the electric and magnetic fields associated to the scalar and vector potentials Φ and $\vec{A}$

$$\vec{\nabla} \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = \vec{0}, \qquad \vec{\nabla} \cdot \vec{B} = 0, \tag{73}$$

precisely the two homogeneous Maxwell equations of electromagnetism. In other words, the general solution to the homogeneous Maxwell equations is given in the form (71) in terms of the scalar and vector electromagnetic potentials Φ and $\vec{A}$ (nevertheless, this still leaves to solve the two inhomogeneous Maxwell equations in which the source terms contribute, namely the scalar charge and vector current densities). This then raises the issue of the uniqueness of these electromagnetic potentials.

Once again because of the second identity in (72), in fact given any two fields $\vec{E}$ and $\vec{B}$ obeying the homogeneous Maxwell equations (73) there exist an infinity of electromagnetic potentials reproducing these fields through the relations (71). Indeed, it is readily checked that the following redefinition of the electromagnetic potentials

$$\Phi'(t,\vec{r}) = \Phi(t,\vec{r}) - \frac{\partial \chi(t,\vec{r})}{\partial t}, \qquad \vec{A}'(t,\vec{r}) = \vec{A}(t,\vec{r}) + \vec{\nabla}\chi(t,\vec{r}), \tag{74}$$

where $\chi(t,\vec{r})$ is an arbitrary function of time and space (possibly subjected to boundary conditions at infinity), leads back to the same electric and magnetic fields as do the potentials Φ and $\vec{A}$. This symmetry transformation represents a huge freedom in the choice of electromagnetic potentials, known as a **local gauge symmetry**. The idea of a local or gauge symmetry entails the idea that the parameters of the symmetry transformation may be not only constants (as in ordinary symmetry transformations; think of a rotation in space of fixed rotation angle and direction), but may be in general arbitrary functions of space and time, thus corresponding to symmetry transformations which differ, though in a continuous fashion, from one point to the next in space or in time. This is certainly an extreme realisation of the concept of symmetry. And in fact this concept of local or gauged symmetries (*i.e.*, made local in time and space) has proved to be central to all the fundamental interactions. As it turns out, the electromagnetic interaction is in fact the physics of the electromagnetic potentials Φ and $\vec{A}$ viewed as scalar and vector fields (in a relativistic context, they are indeed the components of a 4-vector, $A^\mu = (\Phi/c, \vec{A})$, $\mu = 0,1,2,3$, of which the time component, $\mu = 0$, is the scalar potential, and the space components, $\mu = i = 1,2,3$, the vector potential; here c is the velocity of light in vacuum) rather than that of the electric and magnetic fields $\vec{E}$ and $\vec{B}$ which are "only" derived quantities but not the fundamental quantum fields of the electromagnetic

interaction (the photon is the quantum of the electromagnetic potential fields, and not as such that of the electric or magnetic fields). The dynamics of the electromagnetic potential fields Φ and $\vec{A}$ must be formulated in such a manner that it is invariant under the gauge symmetry transformations (74). As a passing remark, let us also mention that it is precisely this gauge symmetry which is the reason why the photon, the quantum of the electromagnetic potential fields, must be exactly massless.

Having identified the gauge symmetry of the scalar and vector potentials, let us also consider how the Lagrange function (58) transforms under a gauge transformation (74). Denoting by L' the Lagrange function in (58) associated to the transformed potentials Φ' and $\vec{A}'$, and by L that associated to the non transformed potentials Φ and $\vec{A}$, one simply has,

$$L' - L = -q\left(-\frac{\partial\chi}{\partial t}\right) + q\dot{\vec{r}}\cdot\vec{\nabla}\chi = \frac{d}{dt}\left(q\chi\right). \tag{75}$$

Hence the two Lagrange functions differ only by a total time derivative. We know that in such a case they share identical equations of motion, and indeed these equations of motion are expressed solely in terms of the electric and magnetic fields which are gauge invariant in the first place. The gauge symmetry of the electromagnetic interaction is thus an example of a symmetry transformation under which the Lagrange function is invariant up to a surface term.

It is also of interest to consider the evolution in time of the energy of the particle for the present system. Knowing the forces to which it is subjected, we may easily identify those forces which develop a nonvanishing power or work, by projecting the forces onto, say, the velocity $\dot{\vec{r}}(t)$ (in the case of an evaluation of the power of the force). Since the magnetic component of the Lorentz force, $q\dot{\vec{r}}\times\vec{B}$, is always perpendicular to the velocity, it is clear that the magnetic field, or this magnetic force never develops any power nor work, and thus does not contribute to the energy balance in the system. Thus only the (total) potential energy $V(\vec{r})$ of the mechanical force(s) as well as the electromagnetic potential energy $q\Phi(t,\vec{r})$ associated to the scalar potential should be considered in combination with the kinetic energy to characterise the total mechanical energy of the particle,

$$E = \frac{1}{2}m\dot{\vec{r}}^2 + q\Phi(t,\vec{r}) + V(\vec{r}). \tag{76}$$

However, in the case that at least one field among the electric or the magnetic fields is not static, namely carries a time dependence, and thus so do also the scalar and vector potentials, one ought to expect that this total mechanical energy of the particle is not conserved (imagine a passing electromagnetic wave, thus setting into motion, or at least a different motion, the particle with otherwise a conserved energy). Indeed, a simple calculation of the rate of change of the total mechanical energy finds

$$\frac{dE}{dt} = q\frac{\partial\Phi}{\partial t} - q\dot{\vec{r}}\cdot\frac{\partial\vec{A}}{\partial t}. \tag{77}$$

Hence indeed, it is only when both the scalar and vector potentials are static, and thus so are also the electric and magnetic fields, namely are time independent, that the total mechanical energy of the particle is a constant of motion.

3 Hamiltonian Dynamics

As a motivation for the first of the definitions given hereafter and laying the basis for the Hamiltonian formulation of dynamical systems, let us just say here that one of the purposes of this formalism is to turn the second order in time differential Euler–Lagrange equations of motion into first order ones, which is *a priori* an advantage when it comes to constructing explicit solutions. However, this comes with the necessity to consider twice as many functions of time to solve for in comparison with the original set of generalised coordinate functions $q^n(t)$ (but on the other hand after all, the Lagrange function already depends on the variables q^n and $\dot{q}^n$), hence the next definition. Let us also mention here in passing that all mathematical studies of chaotic and dynamical systems are best considered within the Hamiltonian formalism, since it allows for powerful mathematical concepts and tools to be brought to bear on difficult issues, leading to the beautiful and still largely to be explored and understood field of symplectic geometry in differential geometry, which, in conjunction with concepts and techniques developed within quantum physics and quantum field theories has seen in recent years important progress and some profound results.

3.1 Conjugate momenta and phase space

Given the system's configuration space parametrised by the coordinates q^n, and its dynamics determined from the Lagrange function $L(q^n, \dot{q}^n)$, by definition the **conjugate momenta**, p_n, of the system, namely a set of variables each of which is conjugate to one of the degrees of freedom, q^n, are defined by the relations,

$$p_n(q^n, \dot{q}^n) = \frac{\partial L(q^n, \dot{q}^n)}{\partial \dot{q}^n}, \qquad n = 1, 2, \ldots, N. \tag{78}$$

Rather than the so-called velocity phase space spanned by the pairs of variables $(q^n, \dot{q}^n)$ $(n = 1, 2, \ldots, N)$, one then considers the (momentum) **phase space**, the $2N$ dimensional manifold spanned by the pairs of variables (q^n, p_n) $(n = 1, 2, \ldots, N)$, namely the configuration space coordinates and their conjugate momenta. In the general case, phase space is the cotangent bundle of the configuration space manifold M_N. However, there are dynamical systems of great interest, both to mathematics and to physics, for which this is not the case, for instance systems of which phase space is compact on account of some nontrivial symmetries.

This definition and concept of conjugate momentum calls for a series of comments.

Comments

1. Based on the definition of the conjugate momenta, one readily notices that the Euler–Lagrange equations of motion may also be written as

$$\dot{p}_n = \frac{\partial L}{\partial q^n}. \tag{79}$$

2. *A priori*, the conjugate momenta are functions of the velocity phase space $(q^n, \dot{q}^n)$, $p_n(q^n, \dot{q}^n)$. But since one would like to trade the velocity phase space for the momentum phase space spanned by the local variables (q^n, p_n), one needs to consider the conditions under which it is possible to express the generalised velocities $\dot{q}^n$ in terms of the phase space variables (q^n, p_n). Thus locally in velocity phase space this requires to consider the relations between the p_n's and the $\dot{q}^n$'s, which in the neighbourhood of any point q^n of configuration space requires to consider the following $N \times N$ square matrix,

$$\frac{\partial p_{n_1}}{\partial \dot{q}^{n_2}} = \frac{\partial^2 L}{\partial \dot{q}^{n_1} \partial \dot{q}^{n_2}}, \tag{80}$$

which thus coincides with the Hessian of the Lagrange function of the system. Consequently in the case of a regular system all such relations may be inverted and all generalised velocities $\dot{q}^n$ expressed as functions of the phase space coordinate variables (q^n, p_n),

$$p_n(q^n, \dot{q}^n) \longleftrightarrow \dot{q}^n(q^n, p_n). \tag{81}$$

As an illustration of this argument in a most simple case, imagine that the dependence of the conjugate momenta on the velocities is purely linear, of the form

$$p_n(q^n, \dot{q}^n) = H_{nn'}(q^n)\dot{q}^{n'}. \tag{82}$$

In such a case it is clear that these relations are invertible provided the $N \times N$ square matrix of coefficients $H_{nn'}(q^n)$ is regular. But this matrix coincides precisely with the quantities $\partial p_n / \partial \dot{q}^{n'}$ considered in the general discussion. In this example, the relations between the p_n's and the $\dot{q}^n$'s are linear, whereas in the general case they are not. But the argument still applies since the problem of inversion is to be considered at each point locally in velocity phase space, and by working in the tangent space to that point precisely similar linear relations are involved of which the coefficients are the entries of the Hessian matrix of $L(q^n, \dot{q}^n)$.

On the other hand, if the Hessian is singular, it then follows that the relations between the p_n's and the $\dot{q}^n$'s may not all be inverted. As we have seen previously, such a situation is characteristic of constrained systems, and indeed this lack of independence of the conjugate momenta p_n then translates into a series of constraints on phase space of the form $\phi(q^n, p_n) = 0$ which must properly be dealt with when considering the Hamiltonian formulation of such systems, which include gauge invariant dynamics, and their subsequent quantisation.

3. Even though two Lagrange functions for a same configuration space which differ by a total time derivative of an arbitrary function of q^n lead to identical equations of motion,

$$L'(q^n, \dot{q}^n) = L(q^n, \dot{q}^n) + \frac{dF(q^n)}{dt} = L(q^n, \dot{q}^n) + \dot{q}^n \frac{\partial F(q^n)}{\partial q^n}, \tag{83}$$

the conjugate momenta associated to each do not coincide,

$$p'_n = p_n + \frac{\partial F(q^n)}{\partial q^n}. \tag{84}$$

Once again, even though this fact does not lead to physical consequences at the classical level, when configuration space has a nontrivial topology such redefinitions of the action lead to observable effects at the quantum level.

3.2 Canonical Hamiltonian and Hamiltonian equations of motion

As a motivation for the next definition, let us consider the differential of the Lagrange function, and aim to make the rôle of the conjugate momenta explicit in that quantity,

$$\begin{aligned} dL(q^n, \dot{q}^n) &= dq^n \frac{\partial L}{\partial q^n} + d\dot{q}^n \frac{\partial L}{\partial \dot{q}^n} \\ &= dq^n \frac{\partial L}{\partial q^n} + d\left[\dot{q}^n \frac{\partial L}{\partial \dot{q}^n}\right] - \dot{q}^n d\frac{\partial L}{\partial \dot{q}^n}, \end{aligned} \tag{85}$$

hence

$$d\left[\dot{q}^n \frac{\partial L}{\partial \dot{q}^n} - L\right] = \dot{q}^n d\frac{\partial L}{\partial \dot{q}^n} - dq^n \frac{\partial L}{\partial q^n}. \tag{86}$$

Since in each of these terms except for the very last one a contribution of $p_n = \partial L/\partial \dot{q}^n$ is now made explicit, let us use the Euler–Lagrange equation to complete the last term as follows,

$$\begin{aligned} d\left[\dot{q}^n p_n - L\right] &= \dot{q}^n dp_n - dq^n \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^n} + dq^n \left[\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^n} - \frac{\partial L}{\partial q^n}\right] \\ &= \dot{q}^n dp_n - dq^n \dot{p}_n + dq^n \left[\dot{p}_n - \frac{\partial L}{\partial q^n}\right], \end{aligned} \tag{87}$$

hence the following definition.

The **canonical Hamiltonian** of the system is the quantity defined hereafter over phase space, constructed through the Legendre transform of the Lagrange function with respect to the conjugate momenta p_n,

$$H_0(q^n, p_n) = \dot{q}^n p_n - L(q^n, \dot{q}^n) \qquad \text{[Legendre transform of } L\text{]}, \tag{88}$$

$$dH_0 = \dot{q}^n dp_n - dq^n \dot{p}_n \left[+dq^n \left(\dot{p}_n - \frac{\partial L}{\partial q^n}\right)\right]. \tag{89}$$

Given the above discussion the following point should be emphasized. It may appear odd that in the definition of the canonical Hamiltonian its dependence is explicitly given to be in terms of the phase space coordinates, (q^n, p_n), rather than the velocity phase space ones, $(q^n, \dot{q}^n)$, since indeed the r.h.s. of the definition in (88) is a combination of quantities which in the general case are functions of the latter variables and not the phase space ones. The truth of the matter is that the calculations leading to (87) show that the quantity defining H_0 is indeed a function of phase space, since its differential is expressible solely in terms of the differentials in dq^n and dp_n only. This means that any dependence of H_0 on $\dot{q}^n$, even in the case of a singular system for which the relations between the p_n's and the $\dot{q}^n$'s may not all be inverted, is through the dependence of H_0 on p_n only and the latter's dependence on the $\dot{q}^n$'s. Irrespective of whether the system is regular or singular, the canonical Hamiltonian always reduces to a function defined over phase space. As we shall see hereafter, the Hamiltonian generates time evolution of the dynamics in phase space. In the case of a singular systems one has to extend the canonical Hamiltonian in order

to induce a time evolution consistent with the constraints (Dirac's analysis of constraints [1, 3]). In the case of a regular system, the canonical Hamiltonian suffices. Only the latter case will thus explicitly be discussed hereafter.

Consequences

1. When one considers classical trajectories which thus obey the Euler–Lagrange equations of motion, the differential of the quantity which defines the canonical Hamiltonian reads

$$dH_0 = \dot{q}^n \, dp_n \, - \, \dot{p}_n \, dq^n. \tag{90}$$

Consequently, by considering separate variations of the canonical Hamiltonian $H_0(q^n, p_n)$ in either one of the q^n's or one of the p_n's, one identifies from this relation the **Hamiltonian equations of motion** of the system for each of its degrees of freedom labelled by $n = 1, 2, \ldots, N$,

$$\dot{q}^n(t) = \frac{\partial H_0(q^n(t), p_n(t))}{\partial p_n}, \qquad \dot{p}_n(t) = -\frac{\partial H_0(q^n(t), p_n(t))}{\partial q^n}, \qquad n = 1, 2, \ldots, N. \tag{91}$$

Note that these are indeed first order in time differential equations. For each of the degrees of freedom $n = 1, 2, \ldots, N$, the second order Euler–Lagrange differential equations have been transformed into twice as many first order Hamiltonian differential equations. These equations have to be supplemented with a choice of boundary conditions. The number of these boundary conditions thus remains the same in both cases, namely two boundary conditions per degree of freedom.

2. **The inverse Legendre transformation or Hamiltonian reduction of phase space**. In the case of regular systems, the definition of the conjugate momenta, $p_n(q^n, \dot{q}^n) = \partial L(q^n, \dot{q}^n)/\partial \dot{q}^n$, may be inverted to express the generalised velocities in terms of the phase space coordinates, $\dot{q}^n(q^n, p_n)$. On the other hand, we now also have, among the Hamiltonian equations of motion, those for the degrees of freedom $q^n(t)$ given in terms of equations for $\dot{q}^n(t)$ in which the r.h.s. is a function of the phase space variables again. Therefore, one may conversely use the first ensemble of Hamiltonian equations of motion to solve for the conjugate momenta in terms of the variables $(q^n, \dot{q}^n)$. Doing so, one is bound to recover the dependence $p_n(q^n, \dot{q}^n)$ obtained from the definition of the conjugate momenta,

$$\dot{q}^n(q^n, p_n) = \frac{\partial H_0(q^n, p_n)}{\partial p_n} \; \longleftrightarrow \; p_n(q^n, \dot{q}^n) = \frac{\partial L(q^n, \dot{q})}{\partial \dot{q}^n}. \tag{92}$$

One may then substitute this expression for the conjugate momenta $p_n(q^n, \dot{q}^n)$ back into the second ensemble of Hamiltonian equations of motion, $\dot{p}_n = -\partial H_0/\partial q_n$, to obtain again the Euler–Lagrange equations of motion of the Lagrangian formulation of the dynamics based on the original Lagrange function $L(q^n, \dot{q}^n)$. Establishing this fact is straightforward and is left to the reader.

3. From the Hamiltonian point of view, phase space defines the **space of states** of the system. Indeed, given initial values for both $q^n(t)$ and $p_n(t)$, the corresponding solution to the Hamiltonian equations of motion defines in a unique manner a specific trajectory in phase space along which the system is evolving in time. Any point on that trajectory then describes the state in which the system is to be found at that time. By extension, phase space is the ensemble of all possible states in which the system may be found. In the Lagrangian formulation, configuration space as such is not sufficient to completely characterise the states of the system, since information either for the velocities or the configurations at different times are also required because of the second order nature of the equations of motion. This identification of phase space with the space of states of the system will extend later to the quantum context in terms of a space of quantum states.

3.3 Phase space dynamics and Poisson brackets

3.3.1 Poisson brackets

Let us now consider an arbitrary observable defined over phase space, $f(q^n, p_n; t)$, which may even possess some explicit time dependence. Most observables are constructed as composite quantities out of the "elementary", "fundamental" or "basic" phase space coordinates (q^n, p_n). As an example think of the total mechanical energy of some ensemble of particles. Clearly, it could be that such an observable includes an explicit time dependence (the previous discussion of the particle in a time dependent background field provides an illustration with as observable the energy), which is the reason why the possibility is allowed in the discussion hereafter.

The rate of change in time in the value of the observable, in other words its equation of motion, is readily established,

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q^n}\dot{q}^n + \frac{\partial f}{\partial p_n}\dot{p}_n = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q^n}\frac{\partial H_0}{\partial p_n} - \frac{\partial f}{\partial p_n}\frac{\partial H_0}{\partial q^n}. \tag{93}$$

This results thus justifies the following definition.

The **Poisson bracket** of two phase space observables f and g is, by definition, the quantity,

$$\{f, g\} = \frac{\partial f}{\partial q^n}\frac{\partial g}{\partial p_n} - \frac{\partial f}{\partial p_n}\frac{\partial g}{\partial q^n}. \tag{94}$$

This definition calls for a series of comments.

Comments

1. As always in these notes unless otherwise specified, whenever indices are repeated in a product, it is implicitly understood they are summed over their whole range of values. Thus in the above definition, the indices n appearing in the partial derivatives are summed over the range $n = 1, 2, \ldots, N$.

2. One should also keep in mind that these Poisson brackets are defined purely in terms of the dependence of the observables on the phase space variables q^n and p_n, irrespective of their dynamics or whatever their time dependence. Thus in fact these Poisson brackets are defined "at equal time", meaning that the arguments q^n and p_n of the observables should be considered at an identical time t for both observables. Even though the notation does not make that explicit, this point has to be kept in mind. In particular, at the quantum level Poisson brackets are put into correspondence with commutation relations of operators, and in the same manner, these commutations relations are then defined "at equal time".

3. In terms of the definition of Poisson brackets, it is clear that the equation of motion for any observable $f(q^n, p_n; t)$ may be expressed more compactly as,

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, H_0\}. \tag{95}$$

Besides their obvious notational advantage, Poisson brackets embody essential features of dynamics and the geometry of phase space for dynamical systems, not to mention their central rôle in the programme of canonical quantisation through the correspondence principle.

As examples of the above general discussion, let us reconsider the Hamiltonian equations of motion for the "elementary" phase space degrees of freedom. By a direct evaluation of the Poisson brackets using their definition, one readily finds

$$\dot{q}^n = \{q^n, H_0\} = \frac{\partial H_0}{\partial p_n}, \qquad \dot{p}_n = \{p_n, H_0\} = -\frac{\partial H_0}{\partial q^n}. \tag{96}$$

These are indeed the correct expressions. Furthermore, let us consider as observable the (canonical) Hamiltonian itself,

$$\frac{dH_0}{dt} = \{H_0, H_0\} = 0. \tag{97}$$

Hence as mentioned previously, having chosen the Lagrange function not to possess any explicit time dependence, it follows that the Hamiltonian of the system is always a constant of motion and conserved. When the evolution parameter t coincides with the physical time, the Hamiltonian coincides with the energy of the system, which is then conserved. The fact that the Hamiltonian coincides with the energy in such circumstances will be illustrated hereafter.

3.3.2 Algebraic properties of Poisson brackets

A direct evaluation of the Poisson brackets for the "elementary" phase space coordinates finds

$$\begin{aligned} \{q^{n_1}, q^{n_2}\} &= 0, & \{q^{n_1}, p_{n_2}\} &= \delta^{n_1}_{n_2}, \\ \{p_{n_1}, q^{n_2}\} &= -\delta^{n_2}_{n_1}, & \{p_{n_1}, p_{n_2}\} &= 0. \end{aligned} \tag{98}$$

These brackets are known as **canonical brackets**, while phase space coordinates obeying such brackets are known as **canonical coordinates**.

Given phase space observables f, g and h, and constants c, c_1 and c_2, it may be shown that Poisson brackets obey the following properties which are purely of an algebraic character,

a) Antisymmetry: $\{f, g\} = -\{g, f\}$.

b) Neutral element: $\{f, c\} = 0$.

c) Linearity: $\{c_1 f + c_2 g, h\} = c_1 \{f, h\} + c_2 \{g, h\}$.

d) Leibnitz rule: $\{fg, h\} = \{f, h\} g + f \{g, h\}$.

e) Jacobi identity: $\{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\} = 0$.

Given these properties and the values (98) of the Poisson brackets for the "elementary" phase space coordinates q^n and p_n, the evaluation of Poisson brackets of any two composite observables becomes a purely algebraic problem, with which one quickly becomes familiar through some solid practice.

Remarks

1. Even though this point will not at all be discussed here, let us only mention that the structure of Poisson brackets with which phase space comes equipped is in fact directly related to the existence of a symplectic geometry on phase space. This fundamental property enables a purely geometric and coordinate free approach to dynamical systems, which has provided profound and important insights into the dynamics of complicated nonlinear systems, and is an essential tool in the mathematical studies of chaotic dynamical systems.

2. One may abstract from the above specific context the algebraic properties of Poisson brackets. There exist other mathematical contexts where identical algebraic properties of a "bracket" arise. In particular, note that the algebra of commutators of matrices, and more generally of linear operators on a vector space, share precisely the same properties as those listed above for Poisson brackets. This remark is at the basis of the correspondence principle between classical and quantum physics, as laid out by P. A. M. Dirac in 1931 in his famous book on quantum mechanics, *The Principles of Quantum Mechanics* (Oxford University Press, 1931), which has known many reprintings. Reading its first few chapters is a must, and a jewel of clarity very much characteristic of most of Dirac's writings. This very point will also be our starting point when addressing the canonical quantisation of a system of which the dynamics is defined through the action principle.

3. There exists a famous theorem due to Darboux, which states that whenever one has a phase space which thus comes equipped with such a bracket structure, namely a symplectic geometry, one may always find locally at each point of phase space a system of canonical coordinates, namely a system of coordinates for which the brackets take the values in (98). In the above discussion starting from the Lagrange function and introducing conjugate momenta, the pairs of phase space coordinates (q^n, p_n) for each $n = 1, 2, \ldots, N$ are always canonical.

3.3.3 The Hamiltonian formulation of dynamical systems

In conclusion, the above discussion has established that the Hamiltonian formulation of any dynamical system is characterised by three essential data, which will be put in direct correspondence with analogous data when considering the quantum dynamics of such a system. These data are:

· space of states:	phase space:	(q^n, p_n)
· algebraic structure: (symplectic geometry)	Poisson brackets:	Canonical brackets $\{q^{n_1}, p_{n_2}\} = \delta^{n_1}_{n_2}$
· time evolution:	Hamiltonian H:	$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, H\}$

In fact, all this information may finally be "encoded" into an action principle but this time defined on phase space rather than configuration space only, in terms of a first-order action (first-order because it depends only linearly on the first order time derivatives of the phase space coordinates). Namely, it is straightforward to check that the Hamiltonian equations of motion for both $\dot{q}^n$ and $\dot{p}_n$ follow from the variational principle (in a weak sense again) applied to the following first-order phase space action,

$$S[q^n, p_n] = \int_{t_i}^{t_f} dt \, \left[\dot{q}^n p_n \, - \, H(q^n, p_n) \, + \, \frac{dF(q^n, p_n)}{dt} \right]. \tag{99}$$

What is remarkable about this action is that all three data listed above play a rôle in its expression. First, there is the space of states through the coordinates (q^n, p_n) parametrising that space. Next, the Poisson bracket structure is directly related[2] to the terms linear in the time derivatives of q^n or p_n (in the above expression, this is the term in $\dot{q}^n p_n$). And finally the generator of time evolution through Poisson brackets, namely the Hamiltonian is explicitly the opposite of the sum of all those terms in the action which do not involve any time derivatives of either q^n or p_n.

In the above action, the function $F(q^n, p_n)$ is arbitrary, and is introduced once again because actions differing by total time derivatives possess identical equations of motion. By adjusting the choice of that total time derivative, alternative and sometimes more convenient forms of the action may be considered. In the case of nontrivial topology in configuration (and phase) space, such redefinitions have physical consequences at the quantum level. Note also that in contradistinction to the Lagrangian formulation, the function $F(q^n, p_n)$ may now be a function of both the q^n's and the p_n's, which allows to specify through the variational principle in a strong sense larger classes of boundary conditions than is possible with the Lagrangian action. Finally, let us just mention that the Hamiltonian formulation of a dynamical system is in a certain sense more "fundamental" than its Lagrangian formulation, especially when singular systems are being considered.

As an example of a redefinition by a total time derivative, consider the function $F(q^n, p_n) = -\frac{1}{2} q^n p_n$, in which case the above action becomes

$$S_2[q^n, p_n] = \int_{t_i}^{t_f} dt \, \left[\frac{1}{2} \left(\dot{q}^n p_n - q^n \dot{p}_n \right) - H(q^n, p_n) \right]. \tag{100}$$

It is interesting to put this expression in relation to that of the action for a charged nonrelativistic particle confined to a plane and subjected to a static and homogeneous magnetic field $\vec{B}$ perpendicular to that plane, namely the system of the "pure Landau problem",

$$S[x, y] = \int_{t_i}^{t_f} dt \, \left[\frac{1}{2} m \left(\dot{x}^2 + \dot{y}^2 \right) \, - \, \frac{1}{2} qB \left(\dot{x} y - x \dot{y} \right) \right], \tag{101}$$

where (x, y) denote cartesian coordinates in the plane. In this expression the choice of gauge for the vector potential is such that $\vec{A}(\vec{r}) = \vec{B} \times \vec{r}/2$, in a three dimensional notation, which is known as the circular or symmetric gauge, since it is covariant under rotations in the plane perpendicular to the magnetic field.

[2] Proof of this statement is not provided here, but may be found in Ref.[3]. In any case, this fact may be established without too much difficulty.

Other choices of gauge, in the form $\vec{A}(t,\vec{r}) = \vec{B}\times\vec{r}/2 + \vec{\nabla}\chi(t,\vec{r})$, $\chi(t,\vec{r})$ being an arbitrary function, are also possible, and simply correspond to redefining the Lagrange function by a total time derivative term with $F(t,\vec{r}) = q\chi(t,\vec{r})$. In the limit of a vanishing mass m (or a ratio B/m growing infinite), this action reduces to

$$\lim_{m\to 0} S_2[x,y] = \int_{t_i}^{t_f} dt \left[-\frac{1}{2}qB\left(\dot{x}y - x\dot{y}\right)\right]. \tag{102}$$

Compared to the above first-order Hamiltonian action, we see that the system is already in Hamiltonian form, with a two dimensional phase space which coincides with the original configuration space of the plane, with canonically conjugate coordinates that may be taken to be, for instance, x and $(-qBy)$, and with an identically vanishing Hamiltonian (had a potential energy term $V(x,y)$ been introduced in the action (101), this potential energy would now play the rôle of the Hamiltonian). Consequently, no classical dynamics survives in this limit (the particle remains pinned to a position, or in actual fact onto the equipotentials of the potential energy $V(x,y)$ were one to be present), while one has the Poisson bracket $\{x,y\} = -1/qB$. Since when quantising the system these brackets become commutation relations and coordinates become operators, this system provides the simplest illustration of a noncommutative geometry in two dimensions, since the cartesian coordinates x and y then do no longer commute.

3.4 Illustrative examples

3.4.1 The nonrelativistic particle

Let us consider the nonrelativistic particle described by the Lagrange function

$$L = \frac{1}{2}m\dot{\vec{r}}^2 - V(\vec{r}). \tag{103}$$

The momentum conjugate to the degrees of freedom $\vec{r}$ is

$$\vec{p} = \frac{\partial L}{\partial \dot{\vec{r}}} = m\dot{\vec{r}}. \tag{104}$$

This quantity thus coincides, in this specific case, with the ordinary linear or velocity momentum of a particle. Clearly, since the velocities may be inverted in terms of the momenta, $\dot{\vec{r}} = \vec{p}/m$, this is also a regular system.

From the general discussion, we know at once that the cartesian components of both the position vector, $\vec{r}$, namely x^i with $i = 1,2,3$, and the conjugate momentum vector, $\vec{p}$, namely p_i, are canonically conjugated coordinates of the phase space $(\vec{r},\vec{p})$ of this system. Hence we have the Poisson brackets (as is customary, only the nonvanishing Poisson brackets are displayed),

$$\left\{x^i, p_j\right\} = \delta^i_j. \tag{105}$$

Furthermore, a direct calculation finds that the canonical Hamiltonian of the system is,

$$H = \dot{\vec{r}}\cdot\vec{p} - L = \frac{1}{2m}\vec{p}^{\,2} + V(\vec{r}), \tag{106}$$

which is seen to coincide with the total mechanical energy of the particle. This is as it should be since the time evolution parameter t is in this case also the physical time. And of course, this energy is a constant of motion for this conservative system.

Having identified the necessary three data for the Hamiltonian formulation of the dynamics, the Hamiltonian equations of motion readily follow, with

$$\dot{\vec{r}} = \{\vec{r},H\} = \frac{1}{m}\vec{p}, \qquad \dot{\vec{p}} = \{\vec{p},H\} = -\vec{\nabla}V(\vec{r}). \tag{107}$$

The first of these vector equations may indeed be solved for $\vec{p}$ in terms of $\dot{\vec{r}}$, $\vec{p} = m\dot{\vec{r}}$, a representation which when substituted into the second Hamiltonian equation of motion recovers the Newton equation for this system,

$$m\ddot{\vec{r}} = -\vec{\nabla}V(\vec{r}) = \vec{F}(\vec{r}). \tag{108}$$

Consequently all the other considerations already developed earlier when this type of system was discussed follow as well. For what concerns the possible conservation of the linear momentum or the angular-momentum now in presence of the potential energy $V(\vec{r})$, one finds

$$\dot{\vec{p}} = -\vec{\nabla} V(\vec{r}) = \vec{F}(\vec{r}), \tag{109}$$

$$\dot{\vec{L}} = \frac{d}{dt}\left[\vec{r}\times\vec{p}\right] = -\vec{r}\times\vec{\nabla}V(\vec{r}) = \vec{r}\times\vec{F}(\vec{r}). \tag{110}$$

Consequently, the linear momentum is conserved only if the particle is free, $\vec{F} = \vec{0}$, while the angular-momentum may be conserved even in the presence of a nonvanishing force provided only it is radial, namely always colinear with the position vector $\vec{r}$. In either of these two situations leading to a conservation law, it is a symmetry law of space which is again at work.

3.4.2 The one dimensional harmonic oscillator

Returning to the one dimensional harmonic oscillator, this is but an example of the previous general discussion particularised to a one degree of freedom system, namely the coordinate $x(t) \in \mathbb{R}$, with

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2. \tag{111}$$

Consequently, it readily follows that

$$p = m\dot{x}, \quad \dot{x} = \frac{1}{m}p, \quad \{x,p\} = 1, \qquad H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2, \tag{112}$$

leading to the equations of motion,

$$\dot{x} = \{x,H\} = \frac{1}{m}p, \quad \dot{p} = \{p,H\} = -m\omega^2 x. \tag{113}$$

From the previous discussion of this system, the solutions are of the form

$$\begin{aligned} x(t) &= \frac{1}{\sqrt{2m\omega}}\left[\alpha_0 e^{-i\omega(t-t_0)} + \alpha_0^* e^{i\omega(t-t_0)}\right], \qquad p(t) = -i\frac{m\omega}{\sqrt{2m\omega}}\left[\alpha_0 e^{-i\omega(t-t_0)} - \alpha_0^* e^{i\omega(t-t_0)}\right], \\ x(t) &= \frac{1}{\sqrt{2m\omega}}\left[\alpha(t) + \alpha^*(t)\right], \qquad\qquad\qquad p(t) = -i\frac{m\omega}{\sqrt{2m\omega}}\left[\alpha(t) - \alpha^*(t)\right], \end{aligned} \tag{114}$$

hence

$$\alpha(t) = \sqrt{\frac{m\omega}{2}}\left[x(t) + \frac{i}{m\omega}p(t)\right], \qquad \alpha^*(t) = \sqrt{\frac{m\omega}{2}}\left[x(t) - \frac{i}{m\omega}p(t)\right]. \tag{115}$$

Clearly, the complex valued integration constant α_0 (and its complex conjugate α_0^*) determines in a unique fashion a trajectory in the phase space of the system. This suggests another point of view on the space of states and the Poisson bracket structure it comes equipped with. Specifying classical solutions to the equations of motion is tantamount to choosing the integration constant α_0. Equivalently, one may say that rather than considering phase space as spanned by the two real coordinates x and p, phase space is spanned by the complex coordinate α which then evolves in time for a specific classical solution according to the dynamics of the system. Hence let us consider the change of variable determined by the coordinate $\alpha(t)$ of which the real and imaginary parts are, up to normalisation factors, the configuration space coordinate $x(t)$ and its conjugate momentum $p(t)$, respectively.

A simple calculation then finds the following Poisson bracket structure,

$$\{\alpha, \alpha^*\} = -i, \tag{116}$$

while the Hamiltonian becomes

$$H = \frac{1}{2}\omega\left[\alpha\,\alpha^* + \alpha^*\,\alpha\right]. \tag{117}$$

In obtaining this latter expression, care has been exercised not to commute the variables α and α^*, since at the quantum level they indeed no longer commute, so that we shall be able to directly take over the above expression for the quantum Hamiltonian of the system.

Given these results, the equation of motion for the complex phase space coordinate is,

$$\dot{\alpha} = \{\alpha, H\} = -i\omega\,\alpha, \qquad \dot{\alpha}^* = \{\alpha, H\} = i\omega\,\alpha^*, \tag{118}$$

of which the solution is obviously,

$$\alpha(t) = \alpha_0\, e^{-i\omega(t-t_0)}, \qquad \alpha^*(t) = \alpha_0^*\, e^{i\omega(t-t_0)}, \tag{119}$$

α_0 being again the necessary integration constant.

3.4.3 The simple pendulum

From a previous discussion, we know the Lagrange function for this system is given as

$$L = \frac{1}{2}m\ell^2\dot{\theta}^2 - mg\ell(1-\cos\theta), \tag{120}$$

for a pendulum of mass m, length ℓ, θ being the angular position of the mass with respect to the downward vertical direction, and also the single degree of freedom of this system. Consequently, we readily obtain,

$$p_\theta = \frac{\partial L}{\partial\dot{\theta}} = m\ell^2\dot{\theta}, \qquad \dot{\theta} = \frac{1}{m\ell^2}p_\theta, \qquad \{\theta, p_\theta\} = 1, \qquad H = \frac{1}{2m\ell^2}p_\theta^2 + mg\ell(1-\cos\theta). \tag{121}$$

The Hamiltonian equations of motion are thus

$$\dot{\theta} = \{\theta, H\} = \frac{1}{m\ell^2}p_\theta, \qquad \dot{p}_\theta = \{p_\theta, H\} = -mg\ell\sin\theta. \tag{122}$$

Reducing the first equation reproduces again the relation $p_\theta = m\ell^2\dot{\theta}$, which upon substitution into the second of these two equations leads back to the Euler–Lagrange equation of the system, namely

$$\ddot{\theta} + \frac{g}{\ell}\sin\theta = 0. \tag{123}$$

3.4.4 The charged nonrelativistic particle in a background electromagnetic field

Using the same notations as in the previous discussion of this system, its Lagrange function is

$$L = \frac{1}{2}m\dot{\vec{r}}^2 - q\Phi(t,\vec{r}) + q\dot{\vec{r}}\cdot\vec{A}(t,\vec{r}) - V(\vec{r}). \tag{124}$$

The conjugate momentum vector is thus,

$$\vec{p} = \frac{\partial L}{\partial\dot{\vec{r}}} = m\dot{\vec{r}} + q\vec{A}(t,\vec{r}), \qquad \dot{\vec{r}} = \frac{1}{m}\left[\vec{p} - q\vec{A}(t,\vec{r})\right]. \tag{125}$$

Note that in this system the conjugate, or canonical momentum $\vec{p}$ **does not** coincide with the ordinary linear or velocity momentum, $m\dot{\vec{r}}$. This is characteristic of systems in the presence of background fields. Hence the Poisson brackets are,

$$\left\{x^i, p_i\right\} = \delta^i_j, \quad i,j = 1,2,3, \tag{126}$$

where x^i and p_i stand for the cartesian coordinates of $\vec{r}$ and $\vec{p}$, respectively.

The determination of the canonical Hamiltonian is straightforward and leads to

$$H = \frac{1}{2m}\left[\vec{p} - q\vec{A}(t,\vec{r})\right]^2 + q\Phi(t,\vec{r}) + V(\vec{r}). \tag{127}$$

The Hamiltonian equations of motion are thus

$$\dot{\vec{r}} = \frac{1}{m}\left[\vec{p} - q\vec{A}(t,\vec{r})\right], \qquad \dot{\vec{p}} = \frac{q}{m}\left[\vec{p} - q\vec{A}(t,\vec{r})\right]^j \cdot \frac{\partial\vec{A}_j(t,\vec{r})}{\partial\vec{r}} - q\vec{\nabla}\Phi(t,\vec{r}) - \vec{\nabla}V(\vec{r}). \tag{128}$$

Once again, it may shown that by using the first of these equations to reduce for the conjugate momentum, and by substituting then its expression into the second of these equations of motion, the Euler–Lagrange equations are recovered in terms of the Lorentz force associated to the scalar and vector potentials $\Phi(t,\vec{r})$ and $\vec{A}(t,\vec{r})$, as well as the force associated to the potential energy $V(\vec{r})$.

Given the explicit time dependence of the Lagrange function, hence also the Hamiltonian, let us consider the time evolution of the latter,

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \{H,H\} = \frac{\partial H}{\partial t} = -\frac{q}{m}\left[\vec{p} - q\vec{A}(t,\vec{r})\right]\cdot\frac{\partial\vec{A}(t,\vec{r})}{\partial t} + q\frac{\partial\Phi(t,\vec{r})}{\partial t} = -q\dot{\vec{r}}\cdot\partial_t\vec{A}(t,\vec{r}) + q\partial_t\Phi(t,\vec{r}). \tag{129}$$

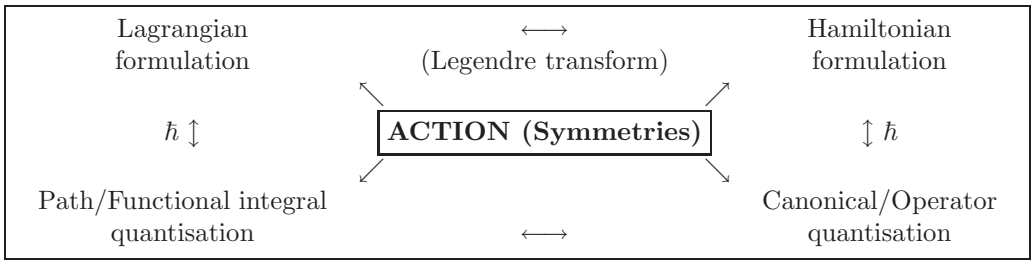
Consequently one has for instance,

$$\frac{d}{dt}\left[\frac{1}{2}m\dot{\vec{r}}^2\right] = q\dot{\vec{r}}\cdot\vec{E}(t,\vec{r}) + \dot{\vec{r}}\cdot\vec{F}(\vec{r}), \tag{130}$$

which is indeed the equation of motion for the kinetic energy of the particle, the r.h.s. being the sum of the powers developed by the electric field $\vec{E}(t,\vec{r})$, on the one hand, and the mechanical force $\vec{F}(\vec{r})$, on the other.

4 Canonical Quantisation

The concept of the action principle is central to the whole discussion and framework within which all observed properties of the fundamental interactions and the elementary particles are being described and understood today. Not only does the action embody in one single expression all the complicated nonlinear equations of motion associated to these dynamical systems, but in fact it also accounts for all the conservation laws through the existence of symmetry transformations of the configurations of these systems which leave the action invariant. Indeed, as follows from Noether's (first) theorem, to be discussed at a later stage, any continuous symmetry of the action directly implies conservation laws, which at the quantum level translate into conserved charges. One famous example is of course the conservation of the electric charge, in fact related to the invariance of the electromagnetic interaction under the local gauge transformations considered already previously, and which extend also to the quantum context and the quantum states of matter degrees of freedom.



In fact, besides the general framework outlined here, the culmination of all the progress made throughout the XX$^{\text{th}}$ century in fundamental physics may well be considered to be the concept of local gauge symmetry, a symmetry realised independently at each point of spacetime though in a continuous fashion. All interactions, whether classical (as still is General Relativity for the gravitational interaction) or quantum (for all other three fundamental interactions) have their properties governed by a gauge symmetry principle. Only the origin of (inertial) mass still escapes that formulation, and is indeed one of the main open problems today for fundamental physics. The Standard Model of the fundamental interactions offers an answer through the Higgs mechanism, and predicts the existence of at least one more scalar particle unobserved so far, known as the higgs. But it remains to be seen through the experiments to be started at the LHC (Large Hadron Collider, CERN, Geneva) whether Nature has not outdone us once again with some far more clever trick than anyone has yet imagined.

Given the general classical frameworks of the Lagrangian and Hamiltonian formulations of dynamics, we are now ready to discuss how dynamical systems, whether mechanical systems or field theories, may be

quantised. The path we shall follow is that of canonical quantisation based on the canonical Hamiltonian formalism, which introduces the fundamental constant of quantum mechanics, namely the reduced Planck constant, $\hbar = h/2\pi \simeq 1.055 \times 10^{-34}$ J·s. Nevertheless, it is possible to also set up path or functional integral representations of quantum matrix elements in which the classical first-order Hamiltonian or even Lagrangian actions appear again explicitly. Such path integral representations thus provide an alternative and complementary approach to quantisation, physically equivalent to the canonical operator approach. Depending on the type of issue to be addressed, one approach is often far more convenient than the other, while they each speak differently to our mathematical and physical intuitions.

The general discussion will be illustrated mostly with the harmonic oscillator, since a great deal may be learned already from so simple a system. However, in a perturbative approach, it is in fact also the harmonic oscillator which lies at the basis of the whole physical interpretation of relativistic quantum field theories as theories of relativistic quantum point particles as being the quantum states of the fields. This latter result is, in certain sense, the fourth revolution of $\mathrm{XX}^{\mathrm{th}}$ century physics, after those of quantum mechanics, special relativity and General Relativity. Merging together quantum mechanics and special relativity leads to relativistic quantum field theory as a dual description of relativistic quantum point particles and relativistic quantum fields.

4.1 The canonical quantisation programme

Hamiltonian dynamics	Correspondence principle (Dirac)	**Quantum dynamics** ($\hbar$)
Canonical formalism		Canonical quantisation
Phase space $(q^n(t), p_n(t))$	$\longleftarrow$ **Space of states** $\longrightarrow$ Representation of	"**Hilbert**" **space**: $\|\psi\rangle$, $\langle\psi\|\chi\rangle = \langle\chi\|\psi\rangle^*$
Poisson brackets $\{A, B\} = C$	**Algebraic** $\longleftarrow$ **structures** $\longrightarrow$	Commutation relations (Equal time, $t = t_0$) $\left[\hat{A}, \hat{B}\right] = i\hbar\hat{C}$
Fundamental brackets $\left\{q^n, q^{n'}\right\} = 0 = \{p_n, p_{n'}\}$ $\{q^n, p_{n'}\} = \delta^n_{n'}$		**Heisenberg algebra**: $\hat{q}^{n\dagger} = \hat{q}^n$, $\hat{p}^\dagger_n = \hat{p}_n$ $\left[\hat{q}^n, \hat{q}^{n'}\right] = 0 = [\hat{p}_n, \hat{p}_{n'}]$ $[\hat{q}^n, \hat{p}_{n'}] = i\hbar\delta^n_{n'}$
Hamiltonian equations of motion	$\longleftarrow$ **Dynamics** $\longrightarrow$	**Schrödinger equation** $i\hbar\frac{d\|\psi,t\rangle}{dt} = \hat{H}_0\,\|\psi, t\rangle$ [Schrödinger picture]
$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \{A, H_0\}$		$i\hbar\frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t), \hat{H}_0\right]$ [Heisenberg picture] $\hat{H}_0$ self-adjoint
Composite observables qp	Example $\longleftrightarrow$	Composite operators [Noether charges]: ordering ambiguities $\hat{q}\hat{p}$, $\hat{p}\hat{q}$, $(\hat{q}\hat{p} + \hat{p}\hat{q})/2$

As indicated in the above Table, to each of the three structures inherent to the Hamiltonian formulation of any classical dynamical system (namely its phase space as the space of states, its Poisson brackets with their algebraic properties also shared, as abstract properties, by the algebra of commutators of linear operators or matrices on a vector space, and finally, its Hamiltonian as the generator of time

evolution through the Poisson brackets for any observable), there correspond, through the **correspondence principle**, three analogous structures for the quantised system. Quantising a system amounts to constructing these three data given their classical counterparts. This requires also the introduction of Planck's (reduced) constant, $\hbar = h/2\pi$. However, there may exist more than a unique quantum system which, in the classical limit $\hbar \to 0$, reproduces a given classical system. It is then a matter of experimental investigations to determine which quantum realisation Nature is "using" for the system. For instance, a rotationally invariant system in space may, at the quantum level, be realised in any of an infinite discrete set of spin values. It is only by measuring the spin value of, say, the electron, that one may determine it to be $1/2$ (in units of $\hbar$). Some people see this multiplicities of quantum realisations as an inconvenience and wish to identify a more restricted quantisation programme leading, given any dynamical system, to a single and unique quantum counterpart. The author of these notes rather sees this issue of multiple quantisations as a virtue, as a riches of opportunities of which Nature certainly makes good "use".

In the quantised system, corresponding to the space of quantum states in which the system may be found and through which it may evolve in time, one now has to consider some "Hilbert" space $\mathcal{H}$, namely a vector space over the complex number and equipped with an inner product which is sesquilinear, hermitian and positive definite. "Hilbert" is here put in between quotation marks for the following reason. In mathematics a **Hilbert space** corresponds to a vector space with all these structures but meeting also a series of further conditions of a more technical character (the Hilbert space of the harmonic oscillator to be discussed hereafter is the example "par excellence" of a genuine Hilbert space). However in physics often it is not possible to satisfy exactly and specifically all the properties characteristic of a Hilbert in the sense of the strict mathematical definition of that word and concept, but physicists proceed nevertheless and achieve nonetheless most impressive results with which Nature seems to be happy (the anomalous magnetic moment $(g-2)$ of the electron has been computed based on QED (Quantum Electrodynamics) to a precision in eleven decimal places, and agrees within that precision with the measured value set by Nature). One such example is that of ordinary plane waves in Euclidean space, corresponding to quantum states of a particle possessing a definite momentum, and the Fourier transformation of (wave) functions. Strictly speaking such plane waves do not span a Hilbert space since they lack normalisability. Yet they define "almost" a Hilbert space (through the theory of distributions and nested Hilbert spaces), and through the use of Dirac's δ-function most often one is "safe" in pretending that the space of states is a Hilbert space.

For the inner product on the space of quantum states, Dirac's "bra-ket" notation is widely used and most convenient (in fact it is based on the important concept of the dual of a vector space, namely the space of linear forms or functions over the vector space taking their values in the number field over which the vector space is constructed, which becomes canonically isomorphic to the vector space itself once the vector space is equipped with a nondegenerate inner product. In that context, the "bra" corresponds in fact to an element of the dual space, and the "ket" to an element of the vector space, with the evaluation of the "bra" vector on the "ket" vector given by the inner product of the two vectors). Let us consider two vectors of the Hilbert space, $|\psi\rangle$ and $|\chi\rangle$, ("ket" vectors) and denote their inner product by the "braket=bra-ket",

$$\langle\psi|\chi\rangle \in \mathbb{C} \tag{131}$$

which is thus a complex number. The statement that the inner product is hermitian means that one has under complex conjugation,

$$\langle\psi|\chi\rangle = \langle\chi|\psi\rangle^*. \tag{132}$$

Note that this implies that the bracket of any state with itself is necessarily a real number, $\langle\psi|\psi\rangle \in \mathbb{R}$. The statement that the inner product is positive definite means that one has both the following properties,

$$||\psi||^2 \equiv \langle\psi|\psi\rangle \geq 0, \qquad \langle\psi|\psi\rangle = 0 \Leftrightarrow |\psi\rangle = 0. \tag{133}$$

Finally, by inner product over $\mathbb{C}$ one means of course that $\langle\psi|\chi\rangle$ is a sesquilinear form, namely linear in the ket vector $|\chi\rangle$ and antilinear in the bra vector $\langle\psi|$,

$$\langle\sum_\alpha c_\alpha\psi_\alpha|\sum_\beta d_\beta\chi_\beta\rangle = \sum_{\alpha,\beta} c_\alpha^*\, d_\beta\, \langle\psi_\alpha|\chi_\beta\rangle. \tag{134}$$

Note that these properties extend to the complex case analogous ones for the ordinary inner product for a vector space over the real numbers. In the latter case, the inner product must be linear in both its

vector arguments and symmetric under the exchange of these, and if positive definite it corresponds to a scalar product. Thus in a Hilbert space over the complex numbers one has, respectively, the properties of sesquilinearity, hermiticity, and finally positive definiteness.

This much having been said, it does not yet determine how to identify the Hilbert space to be associated to a given physical system. How is one to choose the space of quantum states? This is where the second structure comes into action, namely that of the algebraic properties that must be realised on Hilbert space for the physical observables. In the classical theory observables are functions defined over phase space for which one may compute Poisson brackets given the Poisson brackets of the phase space coordinates (q^n, p_n). In the quantised system, observables are represented by, or associated to linear operators acting on the quantum states, which therefore no longer commute with one another in the generic situation. Dirac's proposal for a specific definition of Bohr's correspondence principle is to state, as a correspondence principle indeed, that the commutator of two quantum observables is given by the operator associated to the Poisson bracket of their classical counterparts, up to a factor involving Planck's constant $\hbar$. More specifically, given two classical observables $A(q^n, p_n)$ and $B(q^n, p_n)$, let us denote their Poisson bracket as $C(q^n, p_n)$, $C(q^n, p_n) = \{A(q^n, p_n), B(q^n, p_n)\}$. At the quantum level, one ought to associate to these observables quantum operators acting on the space of quantum states, to be denoted as[3] $\hat{A}$, $\hat{B}$ and $\hat{C}$, respectively. The correspondence principle then states that one should have for the equal time commutation relation of the observables $\hat{A}$ and $\hat{B}$,

$$\left[\hat{A}, \hat{B}\right] = i\hbar\, \hat{C} = i\hbar\, \widehat{\{A, B\}}. \tag{135}$$

Planck's constant thus enters as a normalisation factor, while the imaginary factor "i" is required for reasons to which we come hereafter. Incidentally, this normalisation in terms of Planck's constant $\hbar$ also implies that from now on the action of the system must have the physical dimension of $\hbar$, while furthermore the absolute numerical normalisation of the action also implies specific physical properties for the system. This is most readily seen by considering the commutation relations for the elementary phase space variables.

Thus in particular, associated to the phase space coordinates q^n and p_n, one now has linear operators $\hat{q}^n$ and $\hat{p}_n$ acting on the Hilbert space, which must obey the commutation relations

$$[\hat{q}^n, \hat{p}_{n'}] = i\hbar\, \delta^n_{n'}. \tag{136}$$

Note that in the same way as Poisson brackets are defined at equal time, these commutation relations are defined at equal time, for which we take a specific reference time $t = t_0$ which is not made explicit in the above relations but must be kept in mind.

In fact, given that the inner product is hermitian and evaluated over the complex numbers, one has to specify somewhat further some properties of these quantum observables. At the classical level a physical observable $A(q^n, p_n)$ is real under complex conjugation, $A^*(q^n, p_n) = A(q^n, p_n)$. This property should translate at the quantum level into a corresponding property for the linear operator $\hat{A}$ representing that observable, known as a self-adjoint property[4]. To define this concept, let us first consider an arbitrary linear operator $\hat{A}$ acting on any vector $|\psi\rangle$ of its domain of definition, $\mathrm{dom}\, A$, in Hilbert space as,

$$|\psi\rangle \in \mathrm{dom}\, A: \qquad |\psi\rangle \longrightarrow |\psi'\rangle = \hat{A}\,|\psi\rangle \equiv |\hat{A}\psi\rangle, \tag{137}$$

where the last form for the transformed vector is for later convenience. Consider then any other vector $|\chi\rangle$ in Hilbert space and its inner product with the transformed vector $|\hat{A}\psi\rangle$,

$$\langle\chi|\hat{A}\psi\rangle \equiv \langle\chi|\hat{A}|\psi\rangle. \tag{138}$$

The adjoint operator $\hat{A}^\dagger$ of $\hat{A}$ is then defined to be the operator acting on all the vectors $|\chi\rangle$ of its domain of definition, $\mathrm{dom}\, \hat{A}^\dagger$, as $\hat{A}^\dagger|\chi\rangle \equiv |\hat{A}^\dagger\chi\rangle$ and such that for any vector $|\psi\rangle \in \mathrm{dom}\, \hat{A}$ we have

$$|\psi\rangle \in \mathrm{dom}\, \hat{A}, \quad |\chi\rangle \in \mathrm{dom}\, \hat{A}^\dagger: \qquad \langle\hat{A}^\dagger\chi|\psi\rangle = \langle\chi|\hat{A}\psi\rangle. \tag{139}$$

[3]The "hat" symbol is used to emphasize the fact that one is dealing with quantum operators. However, at a later stage this notation will be dropped, since the meaning should become obvious from the context.

[4]Indeed, as is well known, the spectrum of eigenvalues of a self-adjoint operator is real, as are the values of a real classical observable.

In the case of a finite dimensional vector space equipped with an orthonormal basis for the inner product, the operator $\hat{A}$ is represented by a matrix (namely the matrix elements of $\hat{A}$ in that basis), and the adjoint $\hat{A}^\dagger$ of $\hat{A}$ is then represented by the adjoint of that matrix, namely the complex conjugate of the transposed of the matrix representing $\hat{A}$. If $n, m = 1, 2, \ldots, N$ are indices labelling the orthonormalised basis vectors of a finite N dimensional vector space, the matrix elements of $\hat{A}$ in that basis are a collection of numbers A_{nm} defining a matrix, of which the adjoint, $\left(A^\dagger\right)_{nm} = A^*_{mn}$, namely $A^\dagger = \left(A^{\mathrm{T}}\right)^*$ as matrices, gives the matrix elements of the adjoint operator $\hat{A}^\dagger$ in that same basis.

Given this concept of the adjoint of an operator, an operator $\hat{A}$ is said to be symmetric or hermitian if $\hat{A}$ and $\hat{A}^\dagger$ coincide on the intersection of their domains of definition,

$$\hat{A} \text{ is symmetric or hermitian if } \hat{A} = \hat{A}^\dagger \text{ on } \mathrm{dom}\,\hat{A} \cap \mathrm{dom}\,\hat{A}^\dagger. \tag{140}$$

Indeed, it may be that the two domains are not identical, nor that they would coincide with the full Hilbert space but are only some vector subspaces of the latter. A self-adjoint operator $\hat{A}$ is then such that the domains of definition of both $\hat{A}$ and $\hat{A}^\dagger$ are the full Hilbert space $\mathcal{H}$ while $\hat{A}$ and $\hat{A}^\dagger$ coincide,

$$\hat{A} \text{ is self-adjoint if } \hat{A} = \hat{A}^\dagger \text{ and } \mathrm{dom}\,\hat{A} = \mathcal{H} = \mathrm{dom}\,\hat{A}^\dagger. \tag{141}$$

Hence in principle one has to identify properly the Hilbert space in such a manner that quantum observables $\hat{A}$ and $\hat{B}$ (associated to classical real observables) be represented by self-adjoint operators on $\mathcal{H}$, $\hat{A}^\dagger = \hat{A}$ and $\hat{B}^\dagger = \hat{B}$. On the other hand, given two operators $\hat{A}$ and $\hat{B}$, one finds

$$\left[\hat{A}, \hat{B}\right]^\dagger = -[\hat{A}^\dagger, \hat{B}^\dagger], \tag{142}$$

since

$$[\hat{A}, \hat{B}]^\dagger = \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)^\dagger = \hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger = [\hat{B}^\dagger, \hat{A}^\dagger]. \tag{143}$$

Consequently, in the case of self-adjoint operators as must be quantum observables, we conclude that

$$\left[\hat{A}, \hat{B}\right]^\dagger = -[\hat{A}, \hat{B}]. \tag{144}$$

It is this property which explains why it is necessary to include, besides the normalisation factor specified by Planck's constant $\hbar$, the pure imaginary factor i in the commutation relations (135) and (136).

These concepts having been specified, the correspondence principle thus implies that one should aim to have for all quantum observables $\hat{A}$, $\hat{B}$ and $\hat{C}$ of which the classical counterparts are such that $\{A, B\} = C$, the following equal time commutation relation,

$$[\hat{A}, \hat{B}] = i\hbar\hat{C}, \quad \hat{A}^\dagger = \hat{A}, \quad \hat{B}^\dagger = \hat{B}, \quad \hat{C}^\dagger = \hat{C}. \tag{145}$$

In particular for the elementary phase space variables, one must have a realisation on the Hilbert space $\mathcal{H}$ of the following equal time canonical commutation relations

$$[\hat{q}^n, \hat{p}_{n'}] = i\hbar\,\delta^n_{n'}, \qquad (\hat{q}^n)^\dagger = \hat{q}^n, \quad (\hat{p}_n)^\dagger = \hat{p}_n, \tag{146}$$

defining an algebra known as **the Heisenberg algebra**.

In conclusion, we thus observe that the Hilbert space $\mathcal{H}$ of all quantum states of the system is to be a representation of the algebra of equal commutation relations of the quantum observables, beginning with the elementary phase space canonical coordinates which must obey a Heisenberg algebra. As is the case for the concept of classical phase space which combines both a coordinate parametrisation of that manifold in terms of variables q^n and p_n and the Poisson bracket structure defined for these and given by the canonical brackets in the case of canonical phase space coordinates, in the quantum case the notion of the space of quantum states, namely the Hilbert space of the quantised system, cannot be dissociated from the algebraic structure of equal time commutation relations that must be realised in that Hilbert space. Quantising a system consists precisely in the construction of a Hilbert space for which a given algebra of observables is realised, namely is a representation of that algebra. We shall briefly come back to this issue hereafter.

The last information available on the classical side of the discussion and for which the corresponding structure on the quantum side has not yet been introduced is that pertaining to the dynamics or time evolution of the system generated through the Hamiltonian. Being an observable, there must correspond a self-adjoint quantum operator $\hat{H}$ to the classical Hamiltonian $H(q^n, p_n)$, such that $\hat{H}^\dagger = \hat{H}$. At the quantum level time dependence is thus to be generated by the quantum Hamiltonian $\hat{H}$. Here there are two physically equivalent ways in which this time dependence may be represented. The first is by considering that the quantum state describing the system must evolve in time according to some differential equation in which the Hamiltonian operator contributes, the latter being defined at the initial time $t = t_0$ at which the commutation relations are also specified. Consequently, denoting by $|\psi, t\rangle$ the evolving quantum state, its time evolution is governed by **the Schrödinger equation** in **the Schrödinger picture of quantum physics**,

$$i\hbar \frac{d|\psi, t\rangle}{dt} = \hat{H}|\psi, t\rangle. \tag{147}$$

By **Schrödinger picture**, one means that the time dependence of the dynamics of the quantum system is entirely accounted for through a time dependence of the quantum states only, whereas the quantum operators and observables are defined at the reference time $t = t_0$ at which their equal time commutation relations have been specified.

Alternatively, because of a reason to which we shall return hereafter, time dependence of the dynamics of the quantum system may be accounted for by a time dependence of the operators and observables only, rather than the states, whereas the states are only considered at the reference time $t = t_0$ at which the equal time commutation relations are specified. This choice of representation of the time dependence is called **the Heisenberg picture of quantum physics**. In this picture the time evolution equation of these quantum observables is obtained directly from the classical Hamiltonian equation of motion of an observable through the correspondence principle. For an observable $\hat{A}$ without any explicit time dependence[5], its equal time commutation relation with the Hamiltonian operator $\hat{H}$ must equal $i\hbar$ multiplying the result of the corresponding classical Poisson bracket... which is the first order time variation of the observable, hence leading to **the Schrödinger equation** in **the Heisenberg picture of quantum physics**,

$$i\hbar \frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t), \hat{H}\right]. \tag{148}$$

Note that no time dependence is displayed for the Hamiltonian $\hat{H}$. Indeed, its equation of motion would be $i\hbar\, d\hat{H}/dt = [\hat{H}, \hat{H}] = 0$, so that this operator has no time dependence and keeps its value defined at the reference time t_0 in any case. Note that when the time evolution parameter t coincides with the physical time, $\hat{H}$ measures the energy values of the quantum system, implying thus that energy is conserved even at the quantum level. Later on we shall address the resolution of these Schrödinger equations in terms of the eigenspectrum of the Hamiltonian operator.

This concludes the description of how given a classical dynamics, one may identify a quantum dynamics associated to it through the correspondence principle. All three structures inherent to the classical Hamiltonian formalism find their counterparts in the canonical quantisation of the system. The crucial point of that construction is in fact a construction of the Hilbert space representation of the algebra of quantum observables.

As a matter of fact, it turns out that it is not possible to assign to all classical observables a self-adjoint quantum observable while at the same time obeying all the required commutation relations (a detailed discussion of these difficulties may be found in Ref. [5]). The difficulty is related to the problem of **operator ordering** because variables which at the classical level commute with one another no longer necessarily do so at the quantum level. Take a single degree of freedom system with canonical phase coordinates $\hat{q}$ and $\hat{p}$ hence such that $[\hat{q}, \hat{p}] = i\hbar$. Consider then the classical observable qp. How is one to choose a quantum counterpart? Should it be $\hat{q}\hat{p}$, or $\hat{p}\hat{q}$, or $(\hat{q}\hat{p} + \hat{p}\hat{q})/2$, or yet some other combination of the previous choices? Clearly there is a potential ambiguity. However in this case it is resolved by also requiring that the resulting operator be self-adjoint, and would reduce back to the classical observable when $\hbar \to 0$, namely when $\hat{q}$ and $\hat{p}$ would commute again. The unique choice meeting these requirements

[5]For a classical observable that carries an explicit time dependence, the general quantum equation of motion reads $i\hbar d\hat{A}(t)/dt = i\hbar \partial \hat{A}(t)/\partial t + [\hat{A}(t), \hat{H}]$.

is thus

$$qp \longrightarrow \frac{1}{2}\left[\hat{q}\hat{p} + \hat{p}\hat{q}\right]. \tag{149}$$

However, when it comes to higher order monomials in $\hat{q}$ and $\hat{p}$, the ambiguity remains even when requiring self-adjoint operators, and is even such that if the correspondence principle can be satisfied for the commutation relations for all operators bilinear in the quantities $\hat{q}$ and $\hat{p}$, it cannot be satisfied for all trilinear operators. A specific choice of a subclass of observables for which the correspondence principle remains satisfied has to be made, based on yet other considerations, such as those of symmetries which need to be preserved even at the quantum level (as will be discussed later on, conserved charges related to symmetries are composite observables constructed from the elementary phase space coordinates). However, even the latter is not guaranteed, and when it turns out that there does not exist a quantisation of a system which preserves its classical symmetries, one has a so-called **quantum anomaly**, namely the absence in the quantum system of a classical symmetry, the quantum breakdown of a symmetry.

4.1.1 Illustration: the one dimensional harmonic oscillator

It is time to illustrate the above general considerations with a simple yet nontrivial example, for which we shall take the one dimensional harmonic oscillator. We recall that the classical formulation of that system involves a two dimensional phase space spanned by the canonical and cartesian coordinates (q, p) with the canonical bracket $\{q, p\} = 1$, and a dynamics generated by the Hamiltonian

$$H(q,p) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2. \tag{150}$$

It is also of interest to change variables for the description by combining the two real phase space coordinates into a single complex coordinate,

$$\alpha = \sqrt{\frac{m\omega}{2}}\left[q + \frac{i}{m\omega}p\right], \qquad \alpha^* = \sqrt{\frac{m\omega}{2}}\left[q - \frac{i}{m\omega}p\right], \tag{151}$$

and conversely

$$q = \frac{1}{\sqrt{2m\omega}}\left[\alpha + \alpha^*\right], \quad p = -i\frac{m\omega}{\sqrt{2m\omega}}\left[\alpha - \alpha^*\right]. \tag{152}$$

In terms of this variable and its complex conjugate, the Poisson bracket is

$$\{\alpha, \alpha^*\} = -i, \tag{153}$$

while for the Hamiltonian one finds

$$H = \frac{1}{2}\omega\left[\alpha^*\alpha + \alpha\alpha^*\right], \tag{154}$$

without ever having commuted the variables α and α^* with one another in the calculation.

Applying the correspondence principle of canonical quantisation, the quantised harmonic oscillator is thus determined by the equal time commutation relation of the Heisenberg algebra at the reference time $t = t_0$,

$$[\hat{q}, \hat{p}] = i\hbar, \qquad \hat{q}^\dagger = \hat{q}, \qquad \hat{p}^\dagger = \hat{p}, \tag{155}$$

with a dynamics governed by the quantum Hamiltonian which we may choose to be

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{q}^2. \tag{156}$$

Note that this operator does not suffer an operator ordering ambiguity. The space of quantum states of this system is thus a representation space of that algebra, which needs still to be constructed or identified.

Equivalently however, we may also consider the canonical quantisation of the system based on its description in terms of the complex variable α. The correspondence principle then leads to the equal time commutation relation at the reference time $t = t_0$,

$$[\hat{\alpha}, \hat{\alpha}^\dagger] = i\hbar(-i) = \hbar, \tag{157}$$

as well as the quantum Hamiltonian

$$\hat{H} = \frac{1}{2}\omega \left[\hat{\alpha}^\dagger \hat{\alpha} + \hat{\alpha}\hat{\alpha}^\dagger\right]. \tag{158}$$

In order to avoid having to carry through all the calculations the $\hbar$ factor appearing in the above commutation relation, it is better to absorb it in the normalisation of the operators $\hat{\alpha}$ and $\hat{\alpha}^\dagger$, by dividing each of these operators by $\sqrt{\hbar}$. Let us thus introduce the quantum operators

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{q} + \frac{i}{m\omega}\hat{p}\right], \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{q} - \frac{i}{m\omega}\hat{p}\right], \tag{159}$$

and conversely

$$\hat{q} = \sqrt{\frac{\hbar}{2m\omega}}\left[a + a^\dagger\right], \qquad \hat{p} = -im\omega\sqrt{\frac{\hbar}{2m\omega}}\left[a - a^\dagger\right]. \tag{160}$$

The algebra that the operators a and $a^\dagger$ obey is known as **the Fock algebra**,

$$[a, a^\dagger] = \mathbb{I}, \tag{161}$$

of which the representation in terms of the Fock space is discussed hereafter. In turn, the quantum Hamiltonian now reads

$$\begin{aligned}
\hat{H} &= \frac{1}{2}\hbar\omega\left(a^\dagger a + aa^\dagger\right) \\
&= \frac{1}{2}\hbar\omega\left(a^\dagger a + [a, a^\dagger] + a^\dagger a\right) \\
&= \frac{1}{2}\hbar\omega\left(2a^\dagger a + 1\right) \\
&= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).
\end{aligned} \tag{162}$$

Note that the contribution in $\hbar\omega/2$ to this last expression is of a purely quantum origin, following from the commutator $[a, a^\dagger] = \mathbb{I}$. The reason why in this calculation we wished to bring the operator $a^\dagger$ to the left of the operator a will become clear hereafter, when the construction of a representation of the Fock algebra will have been completed.

4.1.2 Fock space representation

In order to identify a Hilbert space providing a realisation of the Fock space algebra, let us assume there exists some state called the Fock vacuum or ground state (indeed this state turns out to be the ground state or lowest energy state of the quantum harmonic oscillator), denoted $|0\rangle$, and such that being acted on with the operator a it is mapped into the null vector of Hilbert space,

$$a|0\rangle = 0. \tag{163}$$

Furthermore, let us assume at the outset that this state is also normalised, namely $\langle 0|0\rangle = 1$.

Since $|0\rangle$ is annihilated by the operator a, the only other possible action to be considered is that of its adjoint operator, $a^\dagger$, on that state, namely

$$|1\rangle \equiv a^\dagger|0\rangle. \tag{164}$$

The question now is to determine whether this new state is really different from $|0\rangle$, more specifically linearly independent from it and thus defining a new dimension or direction in Hilbert space independent of that associated to $|0\rangle$ as a basis vector, or rather whether the state $|1\rangle$ could simply be linearly dependent of $|0\rangle$ with some complex coefficient λ such that

$$|1\rangle = \lambda\,|0\rangle. \tag{165}$$

In order to establish that this is excluded through a proof by contradiction, let us assume it to be the case, and consider now the action of a again on the state $|1\rangle$. First, independently of the assumption, we have

$$a\,|1\rangle = a\,a^\dagger\,|0\rangle = \left(aa^\dagger - a^\dagger a + a^\dagger a\right)\,|0\rangle = \left([a, a^\dagger] + a^\dagger a\right)|0\rangle = \left(1 + a^\dagger a\right)|0\rangle = |0\rangle, \tag{166}$$

in which in the last step of this series of little expressions use has been made of the fact that the operator a annihilates the vacuum $|0\rangle$. The result $a|1\rangle = |0\rangle$ is thus valid under all circumstances. However, if in addition we were to have also that $|1\rangle = \lambda|0\rangle$, it would follow that

$$a|1\rangle = a\left(\lambda|0\rangle\right) = 0, \tag{167}$$

since a annihilates the state $|0\rangle$. However such a conclusion would be inconsistent with the result $a|1\rangle = |0\rangle$. Therefore we are led to conclude that indeed the state $|1\rangle = a^\dagger|0\rangle$ is a state linearly independent from the vacuum $|0\rangle$.

Through a similar discussion in a recursion procedure, it is possible to establish that the state obtained by acting n times with the operator $a^\dagger$ on the state $|0\rangle$, $(a^\dagger)^n|0\rangle$, is linearly independent from all the states $(a^\dagger)^m|0\rangle$ with $m = n-1, n-2, \ldots, 0$. Consequently, the whole tower of states constructed in this manner out from the Fock vacuum defines a basis of the Hilbert space which they generate and which thus provides a representation of the Fock algebra of the operators a and $a^\dagger$. This space is known as the Fock space representation of the Fock algebra.

In fact, all these states are not only linearly independent for $n = 0, 1, 2, \ldots$ but are mutually orthogonal or perpendicular. Indeed, this follows from the fact, implicit in the above discussion, that the constructed Hilbert space is also equipped with an inner product for which the operators a and $a^\dagger$ are adjoint of one another, and such that $\langle 0|0\rangle = 1$. For instance, one easily finds

$$\langle 0|1\rangle = \langle 0|a^\dagger|0\rangle = \langle 0|a|0\rangle^* = 0. \tag{168}$$

In order that they be also normalised, one defines the normalisation of the Fock space basis vectors, or simply Fock states, as

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n|0\rangle, \qquad n = 0, 1, 2, 3, \ldots \tag{169}$$

Given that choice it does not take much of a calculation using the commutator $[a, a^\dagger] = \mathbb{I}$ repeatedly to check that one has,

$$a|0\rangle = 0, \quad a|n\rangle = \sqrt{n}\,|n-1\rangle, \quad n = 1, 2, \ldots; \qquad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle, \quad n = 0, 1, 2, \ldots, \tag{170}$$

from which it also follows that

$$\langle n|m\rangle = \delta_{nm}, \tag{171}$$

showing that indeed the set of Fock states $\{|n\rangle, n = 0, 1, 2, \ldots\}$ defines an orthonormalised basis of Fock space. Note that the operators a and $a^\dagger$ thus map between successive Fock states. The latter may be viewed as defining a semi-infinite ladder, with $a^\dagger$ moving one step upward on that ladder and a one step downward. The operators a and $a^\dagger$ are thus also known as **the ladder operators**. However a vocabulary more largely used is that of the creation (for $a^\dagger$) and annihilation (for a) operators since, as will become totally clear hereafter, they indeed create of annihilate energy quanta of the system, moving between Fock states differing in a single quantum of excitation in energy.

The action of the ladder operators on the Fock states having been established, it follows that

$$a^\dagger\, a\,|n\rangle = a^\dagger\sqrt{n}|n-1\rangle = n|n\rangle, \qquad aa^\dagger\,|n\rangle = a\sqrt{n+1}|n+1\rangle = (n+1)|n\rangle, \tag{172}$$

hence the Fock algebra is indeed obeyed since it is for each of the Fock basis vectors,

$$[a, a^\dagger]\,|n\rangle = |n\rangle. \tag{173}$$

Note that these results also establish that the Fock states are already the eigenstates of the operator $a^\dagger a$, since $a^\dagger a|n\rangle = n|n\rangle$. Furthermore the eigenvalue n for the Fock state at level n measures the number of times the creation or ladder operator $a^\dagger$ has been applied to the Fock vacuum, namely, as shall be seen later on, the number of quanta present in the system. Hence the operator $N = a^\dagger a$ is often called **the number operator**. Since the Hamiltonian of the system is also expressed in terms of the number operator, $H = \hbar\omega[N + 1/2]$, it follows that the Fock basis also diagonalises the Hamiltonian of the system, hence immediately providing the energy spectrum of the quantised one dimensional harmonic oscillator,

$$H|n\rangle = E_n|n\rangle, \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, 3, \ldots \tag{174}$$

Given this result it is useful to represent all these states in a diagram superposed onto the graph of the potential energy of the system, $V(q) = \frac{1}{2}m\omega^2 q^2$. Measured from the bottom of the harmonic well, the lowest energy state or ground state $|0\rangle$ possesses an energy $\hbar\omega/2$ which is purely of a quantum origin since that contribution originates directly from the Fock algebra commutator $[a, a^\dagger] = \mathbb{I}$. This contribution to the energy is often called **the quantum vacuum energy**. And as quantum excitations of the system, one has the whole ladder of Fock states $|n\rangle$, of which the energies all differ for successive states by the quantum $\hbar\omega$. By adding or removing through some coupling or interaction with the oscillator a certain number of quanta each of energy $\hbar\omega$, it is possible to bring the system into any of the Fock states. The reason why the spectrum is discrete also originates in the Fock algebra commutator. The reason why this discreteness is infinite is because the harmonic potential well has an infinite height. An algebraic reason is that the original Heisenberg algebra, namely also the Fock algebra itself, may only be represented on an infinite dimensional vector space. Indeed, if the representation were to be finite dimensional, taking the trace of either defining commutation relation would lead to an inconsistency of the type $0 = 1$.

We have thus already learned a great deal and acquired some experience with a Hilbert space just from this simple system. Let us use the opportunity to develop some further considerations. Knowing that Fock states define a basis of the full space of quantum states, any state in that space may be expressed as a mixed state of all Fock states $|n\rangle$ through a linear combination of which the coefficients are complex numbers ψ_n,

$$|\psi\rangle = \sum_{n=0}^{\infty} |n\rangle\, \psi_n. \tag{175}$$

Each of the terms $|n\rangle\, \psi_n$ determines the projection of the state $|\psi\rangle$ onto the direction in Hilbert space associated to the Fock state $|n\rangle$, $\psi_n \in \mathbb{C}$ being the component of the state $|\psi\rangle$ with respect to that basis vector. The basis being orthonormalised, the component itself is obtained by the projection of vectors defined by the inner product with which the Hilbert space is equipped, namely

$$\langle n|\psi\rangle = \sum_{m=0}^{\infty} \langle n|m\rangle\, \psi_m = \psi_n. \tag{176}$$

Consequently, we may write

$$|\psi\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|\psi\rangle, \tag{177}$$

which is a very useful relation already as such. However, bringing it into the form

$$|\psi\rangle = \left(\sum_{n=0}^{\infty} |n\rangle\, \langle n|\right) |\psi\rangle, \tag{178}$$

one notices that each of the terms in the brackets on the r.h.s. of this identity, namely $|n\rangle\langle n|$, stands in fact for an operator which is nothing else but the projection operator $\mathbb{P}_n = |n\rangle\langle n|$ onto the direction in Hilbert space defined by the Fock state $|n\rangle$, which has the properties

$$\mathbb{P}_n^2 = \mathbb{P}_n, \qquad \mathbb{P}_n^\dagger = \mathbb{P}_n. \tag{179}$$

Indeed, when acting on any state $|\psi\rangle$, the projector $\mathbb{P}_n = |n\rangle\langle n|$ produces a new vector which is simply the component of $|\psi\rangle$ in the direction of $|n\rangle$,

$$\mathbb{P}_n|\psi\rangle = |n\rangle\langle n|\psi\rangle. \tag{180}$$

It should thus be clear that when summing each of these projectors $\mathbb{P}_n$ over all independent directions in Hilbert space, one then necessarily recovers the identity operator, which is indeed what (178) represents,

$$\mathbb{I} = \sum_{n=0} |n\rangle\, \langle n|. \tag{181}$$

Such a representation of the identity operator is called a **spectral decomposition** (or resolution) of the identity operator, for a reason which is to become totally clear hereafter. As it turns out such an identity

is extremely useful. In the form of (178) it shows how it leads directly to the decomposition of any state in the Fock basis. Likewise for an arbitrary operator $\hat{A}$, we may write directly

$$\hat{A} = \mathbb{I}\,\hat{A}\,\mathbb{I} = \left(\sum_{n=0}^{\infty} |n\rangle\langle n|\right)\,\hat{A}\,\left(\sum_{m=0}^{\infty} |m\rangle\langle m|\right) = \sum_{n,m=0}^{\infty} |n\rangle\,\langle n|\hat{A}|m\rangle\,\langle m|, \tag{182}$$

in which the matrix elements $A_{nm} = \langle n|\hat{A}|m\rangle$ of the (semi-infinite discrete) matrix representing the abstract operator $\hat{A}$ in the Fock basis appear naturally and explicitly. In particular for an operator $\hat{\Lambda}$ which is diagonalised in the Fock basis, and for which the matrix representation is thus diagonal with its eigenvalues $\{\lambda_n, n = 0, 1, 2, \ldots\}$ on the diagonal, the above double sum reduces to a single sum, $\Lambda_{nm} = \langle n|\hat{\Lambda}|m\rangle = \lambda_n\delta_{nm}$, so that

$$\hat{\Lambda} = \sum_{n=0}^{\infty} |n\rangle\,\lambda_n\,\langle n|. \tag{183}$$

Such a decomposition of a diagonal abstract operator in the basis of its eigenvectors is called **the spectral decomposition** (or resolution) of the operator, with the spectrum of its eigenvalues λ_n indeed appearing in between the product of the ket, $|n\rangle$, and bra, $\langle n|$, eigenvectors, or multiplying each of the projection operators $\mathbb{P}_n = |n\rangle\langle n|$ associated to these eigenvectors. The case of the identity operator (181) is the particular situation when all these eigenvalues reduce to unity. As another example, one has the Hamiltonian operator in the Fock state basis which diagonalises it,

$$\hat{H} = \sum_{n=0}^{\infty} |n\rangle\,E_n\,\langle n|, \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right). \tag{184}$$

The above discussion relied mostly on a purely algebraic and abstract approach, and managed to identify most straightforwardly the energy spectrum of the harmonic oscillator. However once the Fock state basis is singled out, abstract operators may also be represented in terms of matrices of which the entries are the matrix elements of the operator in that basis. This then enables a matrix representation of quantum physics, which is essentially how Heisenberg first conceived of the rules of quantum mechanics. As an illustration, knowing how the ladder operators act on the Fock states the values for their matrix elements are readily identified as follows, in the order of increasing $n = 0, 1, 2, \ldots$ values for the Fock states,

$$a: \quad \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}, \qquad a^\dagger: \quad \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}, \tag{185}$$

and as a consequence, we also have the matrix representations of the generators $\hat{q}$ and $\hat{p}$ of the Heisenberg algebra,

$$\hat{q}: \quad \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}, \quad \hat{p}: \quad -im\omega\sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}. \tag{186}$$

Based on these matrices, once again it is possible to check for the commutation relations whether for the Heisenberg algebra, $[\hat{q}, \hat{p}] = i\hbar$, or the Fock algebra, $[a, a^\dagger] = \mathbb{I}$.

4.2 Quantum evolution

As discussed previously, once the Hilbert space appropriate to a given system has been identified or constructed as a representation of the algebra of equal time commutation relations, quantum dynamics is generated by the quantum Hamiltonian through the Schrödinger equation, whether in the Schrödinger or the Heisenberg picture. Hereafter we first discuss certain considerations in relation to the solution to

either of these forms of the Schrödinger equation, to be followed by a demonstration that if the spectrum of the quantum Hamiltonian has been determined, in fact all that there is to know about the dynamics of the quantum system is available explicitly. Determining the energy spectrum amounts to solving the full quantum dynamics.

4.2.1 The Schrödinger and Heisenberg pictures

As discussed previously, in the Schrödinger picture time dependence is totally accounted for through the time dependence of the quantum states, $|\psi, t\rangle$, which have to obey the Schrödinger equation

$$i\hbar \frac{d|\psi, t\rangle}{dt} = \hat{H}\,|\psi, t\rangle, \tag{187}$$

whereas operators are time independent and are considered at the reference time t_0 at which the quantisation programme based on the equal time commutation relations is being developed. Being first order in the time derivative, the general solution to this equation requires a single integration constant or boundary condition, say the value for the state at the reference time $t = t_0$ at which the canonical quantisation and the equal time commutation relations are specified, $|\psi, t_0\rangle$. The solution then reads

$$|\psi, t\rangle = U(t, t_0)\,|\psi, t_0\rangle, \tag{188}$$

where $U(t, t_0)$ is the operator defined by

$$U(t, t_0) = e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}. \tag{189}$$

This operator is known as **the quantum evolution operator** or also **the propagator**[6] of the quantum system. Being defined through the exponential of the Hamiltonian operator through the usual power series expansion,

$$e^{-\frac{i}{\hbar}(t-t_0)\hat{H}} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}(t-t_0)\hat{H} \right)^n, \tag{190}$$

there are certain conditions that may have to be met to ensure the convergence of such an expression. Furthermore, it is crucial that the Hamiltonian $\hat{H}$ also be self-adjoint to guarantee unitarity, namely a time evolution preserving the probabilities of quantum physics. In fact, the quantum evolution operator must obey two important properties,

$$\begin{aligned} \text{Convolution} \quad &: \quad U(t_3, t_2)\,U(t_2, t_1) = U(t_3, t_1), \\ \text{Unitarity} \quad &: \quad U^\dagger(t_2, t_1) = U^{-1}(t_2, t_1)\,(= U(t_1, t_2))\,. \end{aligned} \tag{191}$$

In particular, the property of unitarity of the operator $U(t_2, t_1)$ is indeed required to preserve the probability of a state under time evolution,

$$\langle \psi, t|\psi, t\rangle = \langle \psi, t_0|U^\dagger(t, t_0)\,U(t, t_0)|\psi, t_0\rangle = \langle \psi, t_0|\psi, t_0\rangle. \tag{192}$$

In the Heisenberg picture however, dynamics of the quantum system is totally accounted for through the time dependence of the quantum operators, which have to obey the Schrödinger equation[7]

$$i\hbar \frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t), \hat{H}\right], \tag{193}$$

whereas quantum states are time independent and are considered at the reference time $t = t_0$ at which the canonical quantisation programme is being developed. But since the Schrödinger and Heisenberg pictures of quantum physics are physically equivalent, how are they related? To answer this, let us for instance consider the expectation value in a state $|\psi, t\rangle$ of a given observable $\hat{A}(t_0)$ defined in the Schrödinger picture, $\langle \psi, t|\hat{A}(t_0)|\psi, t\rangle$, the observable being assumed not to carry any explicit time dependence (more generally one could consider expectation values of products of observables). Using the solution to the

[6] Not to be confused with the Feynman propagator of quantum field theory.
[7] In the case of observables that carry no explicit time dependence.

Schrödinger equation, and assuming the state $|\psi, t\rangle$ to have been normalised, $\langle\psi, t|\psi, t\rangle = 1$, we then have for the expectation value of the observable $\hat{A}$ as a function of time t,

$$\langle\hat{A}\rangle(t) \equiv \frac{\langle\psi, t|\hat{A}(t)|\psi, t\rangle}{\langle\psi, t|\psi, t\rangle} = \langle\psi, t_0|U^\dagger(t, t_0)\,\hat{A}(t_0)\,U(t, t_0)|\psi, t_0\rangle = \langle\psi, t_0|\hat{A}(t)|\psi, t_0\rangle, \tag{194}$$

in which we have introduced

$$\hat{A}(t) = U^\dagger(t, t_0)\,\hat{A}(t_0)\,U(t, t_0). \tag{195}$$

Hence, this definition establishes the relation between the Schrödinger and Heisenberg pictures of quantum physics. In particular, this definition also provides the solution to the Schrödinger equation in the Heisenberg picture in terms of the quantum evolution operator $U(t, t_0)$, the operator $\hat{A}(t_0)$ then playing the rôle of an integration constant. Indeed, from the above definition of $\hat{A}(t)$ it readily follows that we have

$$i\hbar\frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t), \hat{H}\right], \tag{196}$$

which is indeed the relevant Schrödinger equation when the quantum observable $\hat{A}$ does not possess any explicit time dependence. The quantum evolution operator is thus central in solving the Schrödinger equation whatever the picture of quantum physics being used.

4.2.2 Diagonalisation of time evolution

Let us now assume that the eigenspectrum of the Hamiltonian operator $\hat{H}$ has been determined (which, in practice, is an extremely difficult problem for any system with the slightest relevance to physical reality),

$$\hat{H}\,|E_m\rangle = E_m\,|E_m\rangle, \tag{197}$$

where the notation is meant to be schematic. In general the index m stands for a multi-index some of which components could even take values in a continuous rather than a discrete set. Furthermore we assume all the eigenstates $|E_m\rangle$ to have been orthonormalised,

$$\langle E_m|E_{m'}\rangle = \delta_{mm'}. \tag{198}$$

Consequently, one has the spectral decomposition of the identity operator

$$\mathbb{I} = \sum_m |E_m\rangle\,\langle E_m|, \tag{199}$$

with in particular, when applied onto any diagonal operator in the basis $|E_m\rangle$, a similar spectral decomposition, such as for instance

$$\hat{H} = \sum_m |E_m\rangle\,E_m\,\langle E_m|, \tag{200}$$

$$U(t_2, t_1) = \sum_m |E_m\rangle\,e^{-\frac{i}{\hbar}(t_2-t_1)\,E_m}\,\langle E_m|. \tag{201}$$

Given this last decomposition of the evolution operator, the solution to the Schrödinger equation whether in the Schrödinger or the Heisenberg pictures is (in the latter case again for an operator that carries no explicit time dependence),

$$|\psi, t\rangle = \sum_m |E_m\rangle\,e^{-\frac{i}{\hbar}(t-t_0)\,E_m}\,\langle E_m|\psi, t_0\rangle, \tag{202}$$

$$\hat{A}(t) = \sum_{m,m'} |E_m\rangle\,e^{\frac{i}{\hbar}(t-t_0)E_m}\,\langle E_m|\hat{A}(t_0)|E_{m'}\rangle\,e^{-\frac{i}{\hbar}(t-t_0)E_{m'}}\,\langle E_{m'}|. \tag{203}$$

Consequently, if the eigenspectrum of the Hamiltonian operator is completely known, the entire dynamical time evolution of the quantum system is also determined.

4.2.3 Illustration: the one dimensional harmonic oscillator

Since the energy spectrum of the harmonic oscillator is

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \qquad n = 0, 1, 2, \ldots, \tag{204}$$

the above general discussion translates into the following simple terms. Based on the spectral decomposition of the unit operator in terms of the Fock states $|n\rangle$,

$$\mathbb{I} = \sum_{n=0}^{\infty} |n\rangle\,\langle n|, \tag{205}$$

one simply obtains for the quantum evolution operator

$$U(t_2, t_1) = \sum_{n=0}^{\infty} |n\rangle\, e^{-\frac{i}{\hbar}(t_2-t_1)\hbar\omega(n+1/2)}\,\langle n| = e^{-\frac{1}{2}i\omega(t_2-t_1)} \sum_{n=0}^{\infty} |n\rangle\, e^{-in\omega(t_2-t_1)}\,\langle n|. \tag{206}$$

Based on that spectral decomposition, it follows that for quantum states in the Schrödinger picture one has for the solutions to the Schrödinger equation,

$$|\psi, t\rangle = U(t, t_0)\,|\psi, t_0\rangle = e^{-\frac{1}{2}i\omega(t-t_0)} \sum_{n=0}^{\infty} |n\rangle\, e^{-in\omega(t-t_0)}\,\langle n|\psi, t_0\rangle. \tag{207}$$

For what concerns the Heisenberg picture, let us consider as observables the ladder operators as well as $\hat{q}$ and $\hat{p}$. Given the definition (195) of the time dependence of operators in the Heisenberg picture, one needs to use one of the Baker–Campbell–Hausdorff formulae,

$$e^A\, B\, e^{-A} = B + [A, B] + \frac{1}{2!}\,[A, [A, B]] + \ldots + \frac{1}{n!}\,[A, [A, [\cdots, [A, [A, B]]\cdots]] + \ldots \tag{208}$$

Applying this expression to

$$a(t) = e^{\frac{i}{\hbar}(t-t_0)\hat{H}}\, a(t_0)\, e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}, \tag{209}$$

and using the fact that

$$\left[\frac{i}{\hbar}(t-t_0)\hat{H}, a(t_0)\right] = i\omega(t-t_0)\left[a^\dagger a, a\right] = -i\omega(t-t_0), \tag{210}$$

it follows that

$$a(t) = a(t_0)\, e^{-i\omega(t-t_0)}, \tag{211}$$

and thus also

$$a^\dagger(t) = a^\dagger(t_0)\, e^{i\omega(t-t_0)}. \tag{212}$$

Note that these time dependencies are precisely those of the classical solutions as well, in terms of the coefficients denoted $\alpha(t)$ and $\alpha^*(t)$ as introduced previously but differing from $a(t)$ and $a^\dagger(t)$ only by a normalisation factor of $\sqrt{\hbar}$. Furthermore, the time dependence of the position and conjugate momentum operators then also follows,

$$\hat{q}(t) = \sqrt{\frac{\hbar}{2m\omega}}\left[a(t_0)\, e^{-i\omega(t-t_0)} \,+\, a(t_0)\, e^{i\omega(t-t_0)}\right], \tag{213}$$

$$\hat{p}(t) = -im\omega\sqrt{\frac{\hbar}{2m\omega}}\left[a(t_0)\, e^{-i\omega(t-t_0)} \,-\, a(t_0)\, e^{i\omega(t-t_0)}\right]. \tag{214}$$

Once again these time dependencies coincide with those of the classical solutions to the Hamiltonian equations of motion. Of course this is as expected given that the Schrödinger equation for a quantum observable in the Heisenberg picture is in correspondence, through canonical quantisation, with the Hamiltonian equation of motion for the classical counterpart of that observable. In particular, the configuration space operator $\hat{q}(t)$ in the Heisenberg picture obeys precisely, as an operator now, the original Euler–Lagrange equation of motion of the system,

$$\left[\frac{d^2}{dt^2} \,+\, \omega^2\right]\,\hat{q}(t) = 0. \tag{215}$$

This observation serves as a basis for a heuristic argument showing that any theory of relativistic quantum point particles is necessarily also a theory of relativistic quantum fields [1].

4.3 Representations of the Heisenberg algebra I

Within the context of the harmonic oscillator, starting from the Heisenberg algebra, $[\hat{q}, \hat{p}] = i\hbar$, of the phase space observables, we introduced the creation and annihilation operators $a^\dagger$ and a in terms of which an abstract Hilbert space representation of the Fock algebra was constructed, as well as the Fock basis identified within it, which enabled directly the diagonalisation of the Hamiltonian of the harmonic oscillator. Hence the Fock space representation of the Fock algebra already provides in fact an abstract representation of the Heisenberg algebra as well, through the relations

$$\hat{q} = \sqrt{\frac{\hbar}{2m\omega}} \left[a + a^\dagger\right], \qquad \hat{p} = -im\omega\sqrt{\frac{\hbar}{2m\omega}} \left[a - a^\dagger\right]. \tag{216}$$

Furthermore, given the Fock basis in that Hilbert space, operators acquire a matrix representation which obeys the same commutation relations once again. In other words, there also exists a matrix representation, albeit in terms of semi-infinite matrices, of the same abstract algebraic structure defining the space of quantum states of the harmonic oscillator. This raises the issue of finding all possible representations of the Heisenberg algebra, beginning with a single degree of freedom system. For a finite number N of degrees of freedom, the Heisenberg algebra is the N-fold tensor product of the Heisenberg algebra for a single degree of freedom, hence so is its representation space. Let us thus restrict to the Heisenberg algebra for a single degree of freedom.

In the case that the classical phase space (q, p) is simply Euclidean (and thus by extension for any Euclidean configuration space of any dimension N with cartesian coordinates q^n), there exists a famous result due to von Neumann and Stone stating that up to unitary transformations in Hilbert space (indeed quantum states are defined up to an arbitrary overall unitary transformation which does not affect physical observations of the quantum dynamics), there exists a single representation of the Heisenberg algebra (a derivation of this result may be found for example in Refs. [3, 6]). In other words, the two representations that have already been constructed are but two different realisations of a common underlying abstract Hilbert space realisation of the Heisenberg algebra.

However, let us just state here that if the configuration space possesses a nontrivial topology such that there exist noncontractible cycles within it (namely, when its first homotopy group is nontrivial), then there exists in fact an infinity of unitarily inequivalent representations of the Heisenberg algebra, labelled by U(1) holonomies around the noncontractible cycles [6]. Furthermore, the discussion presented hereafter may also be extended to curved configuration space manifolds, but only the case of Euclidean geometry will be detailed here.

4.3.1 Configuration and momentum space representations

Let us thus consider as configuration space the real line $\mathbb{R}$, with $q \in \mathbb{R}$, and its momentum conjugate p also spanning that range of values, $p \in \mathbb{R}$. Given this configuration and phase space Euclidean geometry, one may then establish the existence of two representations of the Heisenberg algebra in terms of complex functions of q in one case and of p in the other case, hence known as **configuration** and **momentum space wave function representations** of the Heisenberg algebra. These two possibilities correspond to what is usually introduced to define quantum mechanics in a first course on the subject. Here these considerations follow a discussion of the representation theory of the abstract Heisenberg algebra, which arises whatever dynamical system is being quantised. Note well that our discussion thus does not assume implicitly the dynamics of the harmonic oscillator. The discussion to be developed hereafter is totally independent from any dynamical consideration, but is purely kinematical in character.

a) *The configuration space wave function representation*

Let us assume there exists in Hilbert space a basis of position eigenstates, namely states $|q\rangle$ labelled by the eigenvalues of the configuration space or position operator $\hat{q}$ with a spectrum spanning all of $\mathbb{R}$,

$$\hat{q}\,|q\rangle = q\,|q\rangle, \qquad q \in \mathbb{R}. \tag{217}$$

Furthermore, let us assume that these states are normalised, while they may be assumed to be orthogonal

since $\hat{q}$ is self-adjoint[8], $\hat{q}^\dagger = \hat{q}$. Consequently, we have the inner products

$$\langle q|q'\rangle = \delta(q - q'), \tag{218}$$

where $\delta(q - q')$ is the Dirac δ-function. The main property of the δ-"function" (strictly speaking it is a distribution, and its evaluation has to be understood inside an integral where it is multiplied with a test function for the purpose of evaluating the integral) is that given any function $f(x)$ of a single variable, the δ-function $\delta(x - a)$ is such that

$$\int_{-\infty}^{+\infty} dx\, f(x)\delta(x - a) = f(a). \tag{219}$$

In other words, the δ-function is analogous to the Kronecker δ_{nm} symbol in which the set of integers would have been closed into the set of real numbers by having grown ever more dense on the real line. The δ-function thus vanishes whenever its argument is nonvanishing, whereas it takes an infinite value when its argument vanishes but in such a manner that one has a finite value thus normalised to unity when the δ-function is evaluated inside the following integral[9] (again in the same way that when summing the Kronecker δ_{nm} symbol over all the range of values of one of its indices it returns the unit value),

$$\int_{-\infty}^{+\infty} dx\, \delta(x - a) = 1. \tag{220}$$

Given these remarks, it should clear that the condition (218) indeed expresses the orthonormality of the basis $|q\rangle$ of the position eigenstates of $\hat{q}$.

Given this basis, once again one may consider the sum over all basis vectors of the associated projection operators $|q\rangle\langle q|$, which is to reproduce the identity operator,

$$\mathbb{I} = \int_{-\infty}^{+\infty} dq\, |q\rangle\, \langle q|. \tag{221}$$

That this expression is indeed consistent may easily be checked by applying it onto any of the position eigenstates, $|q\rangle = \mathbb{I}|q\rangle$,

$$\mathbb{I}|q\rangle = \int_{-\infty}^{+\infty} dq'\, |q'\rangle\, \langle q'|q\rangle = \int_{-\infty}^{+\infty} dq'\, |q'\rangle\, \delta(q - q') = |q\rangle, \tag{222}$$

indeed as it should. Being true for all basis vectors $|q\rangle$, by linearity in Hilbert space it is true for any quantum state, hence (221) does apply.

But then for any quantum state $|\psi\rangle$ we have

$$|\psi\rangle = \mathbb{I}|\psi\rangle = \int_{-\infty}^{+\infty} dq\, |q\rangle\, \langle q|\psi\rangle = \int_{-\infty}^{+\infty} dq\, |q\rangle\, \psi(q). \tag{223}$$

This identity thus provides the decomposition of the state $|\psi\rangle$ in the basis $|q\rangle$ in terms of its components $\langle q|\psi\rangle$ which define **the configuration space wave function** of the state $|\psi\rangle$,

$$\psi(q) = \langle q|\psi\rangle, \tag{224}$$

indeed a complex valued quantity.

As a consequence, it also becomes possible to determine the representation of the operators $\hat{q}$ and $\hat{p}$ acting on any state $|\psi\rangle$ through their matrix element in the configuration space basis $|q\rangle$. A simple analysis using the Heisenberg algebra[10] then finds

$$\langle q|\hat{q}|\psi\rangle = q\, \langle q|\psi\rangle = q\, \psi(q), \qquad \langle q|\hat{p}|\psi\rangle = -i\hbar \frac{d\psi(q)}{dq}. \tag{225}$$

[8]Indeed, a self-adjoint operator is necessarily diagonalisable and such that its eigenvectors for distinct eigenvalues are orthogonal. These results are well known for finite dimensional matrices, and extend to operators on a Hilbert space.

[9]Even though the δ-function is infinite for a vanishing argument, the latter value is a point of zero measure in the integral so that it remains possible that the integral be finite. One may also introduce different approximations to the δ-function through a limit procedure, such as in the Gaussian representation $\delta(x - a) = \lim_{\epsilon \to 0} \frac{1}{\sqrt{2\pi\epsilon}}\, e^{-\frac{1}{2\epsilon}(x-a)^2}$.

[10]See for instance Ref. [3], even though there exist alternative derivations of these results, all of which have as starting point the Heisenberg algebra commutator.

In other words, when using the configuration space wave function representation $\psi(q)$ of quantum states, the action of the quantum operators $\hat{q}$ and $\hat{p}$ is through multiplication by q in the first case, and differentiation with respect to q as well as multiplication by $(-i\hbar)$ in the second case, of the wave function $\psi(q)$. That these operations now acting on functions (which is indeed a set spanning a vector space over the complex numbers) define a representation of the abstract Heisenberg algebra follows from their commutator as differential operators,

$$\left[q, -i\hbar\frac{d}{dq}\right] = i\hbar. \tag{226}$$

Furthermore the inner product of quantum states, $\langle\psi|\chi\rangle$, then also translates into an integral expression in terms of the associated configuration space wave functions, which indeed defines an inner product over the space of functions possessing all the required properties for a Hilbert space. Namely, using once again the spectral decomposition of the identity operator (221), it follows

$$\langle\psi|\chi\rangle = \langle\psi|\mathbb{I}|\chi\rangle = \langle\psi|\int_{-\infty}^{+\infty} dq|q\rangle\langle q|\chi\rangle = \int_{-\infty}^{+\infty} dq\,\langle\psi|q\rangle\,\langle q|\chi\rangle = \int_{-\infty}^{+\infty} dq\,\psi^*(q)\,\chi(q), \tag{227}$$

with $\psi(q) = \langle q|\psi\rangle$ and $\chi(q) = \langle q|\chi\rangle$. The abstract Hilbert space of the Heisenberg algebra is thereby represented in terms of the space $L^2(\mathbb{R}, dq)$ of square integrable configuration space wave functions,

$$\int_{-\infty}^{+\infty} dq\,|\psi(q)|^2 \,<\, \infty, \tag{228}$$

so that they may be divided by their finite norm and be of norm unity for the inner product (227), while the abstract operators $\hat{q}$ and $\hat{p}$ are then represented by the functional operators as specified above.

b) *The momentum space wave function representation*

It should be quite obvious that a story similar to the one above also applies to a momentum space wave function representation of the Heisenberg algebra. For instance, under the exchange of both operators $\hat{q}$ and $\hat{p}$ and a change of sign in $\hbar$ (a "duality" transformation in a certain sense), the Heisenberg algebra remains invariant. Consequently all the above considerations and results translate into corresponding ones for a momentum space wave function representation.

For that purpose, let us again assume that, since the operator $\hat{p}$ is self-adjoint, there exists a basis of momentum eigenstates $|p\rangle$ of which the eigenspectrum is the real line which is also the range of the classical conjugate momentum variable in phase space,

$$\hat{p}\,|p\rangle = p\,|p\rangle, \qquad p \in \mathbb{R}. \tag{229}$$

Even though this leaves open still the phase of the states $|p\rangle$, their normalisation may be specified once again through their inner products, which should be proportional to the Dirac δ-function in momentum space this time, and for which we choose again a normalisation which is that of an orthonormalised basis,

$$\langle p|p'\rangle = \delta(p - p'). \tag{230}$$

Consequently the spectral decomposition of the identity operator reads

$$\mathbb{I} = \int_{-\infty}^{+\infty} dp\,|p\rangle\,\langle p|, \tag{231}$$

as is confirmed by applying this identity onto any of the the momentum eigenstates $|p\rangle$ as was discussed above for the configuration space eigenbasis. In particular, abstract quantum states $|\psi\rangle$ are then represented in terms of a complex wave function over momentum space[11], $\widetilde{\psi}(p)$, which specifies the components of the state $|\psi\rangle$ in the momentum eigenbasis,

$$|\psi\rangle = \int_{-\infty}^{+\infty} dp\,|p\rangle\,\langle p|\psi\rangle = \int_{-\infty}^{+\infty} dp\,|p\rangle\,\widetilde{\psi}(p), \qquad \widetilde{\psi}(p) = \langle p|\psi\rangle. \tag{232}$$

[11]The tilde above the wave function symbol in momentum space is included to avoid confusing that wave function with the configuration space one.

Furthermore the abstract operators $\hat{q}$ and $\hat{p}$ now also acquire realisations in terms of functional operators acting on the momentum wave function, through

$$\langle p|\hat{q}|\psi\rangle = +i\hbar\frac{d\widetilde{\psi}(p)}{dp}, \qquad\qquad \langle p|\hat{p}|\psi\rangle = p\,\widetilde{\psi}(p). \tag{233}$$

Namely $\hat{q}$ is now represented by the derivative of the wave function with respect to p and multiplied by $(i\hbar)$ while $\hat{p}$ is realised simply as multiplication of the wave function by p. In particular, one may check that these two functional operators do indeed obey the Heisenberg algebra on the vector space of momentum wave functions $\widetilde{\psi}(p)$,

$$\left[i\hbar\frac{d}{dp}, p\right] = i\hbar. \tag{234}$$

The vector space of such wave functions is equipped with an inner product which possesses all the required properties of sesquilinearity, hermiticity and positive definiteness. By making use once again of the spectral decomposition of the identity operator in momentum space, the inner product of any two states $|\psi\rangle$ and $|\chi\rangle$ represented by their momentum wave functions $\widetilde{\psi}(p)$ and $\widetilde{\chi}(p)$ is simply

$$\langle\psi|\chi\rangle = \int_{-\infty}^{+\infty} dp\,\langle\psi|p\rangle\,\langle p|\chi\rangle = \int_{-\infty}^{+\infty} dp\,\widetilde{\psi}^*(p)\,\widetilde{\chi}(p). \tag{235}$$

In particular, and to be precise, the actual Hilbert space (in the strict mathematical sense) consists of all those square integrable wave functions, namely those of finite norm so that the associated states may be normalised to unity,

$$||\psi||^2 = \langle\psi|\psi\rangle = \int_{-\infty}^{+\infty} dp|\widetilde{\psi}(p)|^2 < \infty. \tag{236}$$

c) *Change of basis*

Given the statement that, up to unitary transformations (namely in the case of each of the above two wave function representations, the fact that the position or momentum eigenstates, hence also the wave functions are only defined up to local phase factors), there exists a single representation of the abstract Heisenberg algebra, we know that the Hilbert spaces realised by the above two wave function representations are in fact identical. In other words, the two bases of vectors, $|q\rangle$ and $|p\rangle$, that have been identified provide different bases within the same abstract Hilbert space as a vector space. Since both are orthonormalised bases, there should exist a unitary transformation relating these two bases and transforming the two classes of wave function representations for a same abstract quantum state $|\psi\rangle$. By analogy with the situation for an ordinary finite dimensional vector space over the real numbers, it is clear that knowing the decomposition of one set of basis vectors in terms of the other basis is all that is required to determine the unitary transformation. But such a decomposition amounts to determining the projections of one set of basis vectors onto those of the other set, namely in the present case determine the quantities

$$\langle q|p\rangle, \qquad \langle p|q\rangle = \langle q|p\rangle^*. \tag{237}$$

For instance, $\langle q|p\rangle$ stands for the configuration space wave function of the momentum eigenstate $|p\rangle$, namely a function of q for a fixed value of p. In order to determine this function, let us establish a differential equation for it by considering the matrix element

$$\langle q|\hat{p}|p\rangle = p\,\langle q|p\rangle, \tag{238}$$

which indeed produces the sought for function $\langle q|p\rangle$. On the other hand since that matrix element also defines the realisation of the abstract operator $\hat{p}$ in the configuration space representation, one has

$$\langle q|\hat{p}|p\rangle = -i\hbar\frac{d\langle q|p\rangle}{dq}. \tag{239}$$

We have thus established the differential equation

$$\frac{d\langle q|p\rangle}{dq} = \frac{i}{\hbar}\,p\,\langle q|p\rangle, \tag{240}$$

of which the solution is

$$\langle q|p\rangle = N\, e^{\frac{i}{\hbar}qp}, \tag{241}$$

N being some complex normalisation factor. However one should have, for instance,

$$\delta(q-q') = \langle q|q'\rangle = \int_{-\infty}^{+\infty} dp\, \langle q|p\rangle\, \langle p|q'\rangle = |N|^2 \int_{-\infty}^{+\infty} dp\, e^{\frac{i}{\hbar}p(q-q')} = 2\pi\hbar|N|^2\, \delta(q-q'). \tag{242}$$

In conclusion, up to an arbitrary phase factor set to unity here, we have $N = (2\pi\hbar)^{-1/2}$, and finally

$$\langle q|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{i}{\hbar}qp}, \qquad \langle p|q\rangle = \langle q|p\rangle^* = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-\frac{i}{\hbar}qp}. \tag{243}$$

Having established the change of bases for the position and momentum eigenstates, let us turn to the unitary transformation of the wave functions themselves for an arbitrary state $|\psi\rangle$. Using once again the spectral decompositions of the identity operator, one finds

$$\widetilde{\psi}(p) = \langle p|\psi\rangle = \int_{-\infty}^{+\infty} dq\, \langle p|q\rangle\, \langle q|\psi\rangle = \int_{-\infty}^{+\infty} \frac{dq}{\sqrt{2\pi\hbar}}\, e^{-\frac{i}{\hbar}qp}\, \psi(q), \tag{244}$$

$$\psi(q) = \langle q|\psi\rangle = \int_{-\infty}^{+\infty} dp\, \langle q|p\rangle\langle p|\psi\rangle = \int_{-\infty}^{+\infty} \frac{dp}{\sqrt{2\pi\hbar}}\, e^{\frac{i}{\hbar}qp}\, \widetilde{\psi}(p). \tag{245}$$

In these expressions one recognises the Fourier transformation formulae of a complex function. Hence configuration and momentum wave functions are related through the above Fourier transforms, while this connection between the two finds its origin in the abstract Heisenberg algebra which underlies the whole discussion. In the pure imaginary exponential factors for $\langle q|p\rangle$ and $\langle p|q\rangle$ one also recognises the ordinary "plane wave" factors, which have to do with the behaviour of quantum states under translations in phase space in either q or p, namely a symmetry group. We shall thus come back to this point when discussing symmetries and the (first) Noether theorem.

<u>Remark</u>: The Heisenberg uncertainty relation

As already mentioned, given an operator $\hat{A}(t_0)$ and a quantum state $|\psi,t\rangle$ (both, say, in the Schrödinger picture), the expectation value of that observable is defined as

$$\langle\hat{A}\rangle(t) = \frac{\langle\psi,t|\hat{A}(t_0)|\psi,t\rangle}{\langle\psi,t|\psi,t\rangle}. \tag{246}$$

In the case of the Heisenberg operators $\hat{q}$ and $\hat{p}$, let us then introduce the following quantities. First the expectation values or mean values for both the position and the conjugate momentum of the state,

$$\bar{x}(t) = \langle\hat{x}\rangle(t), \qquad \bar{p}(t) = \langle\hat{p}\rangle(t), \tag{247}$$

and next the mean values for the variations from these means,

$$(\Delta x)^2\,(t) = \langle(\hat{x}-\bar{x})^2\rangle(t), \qquad (\Delta p)^2\,(t) = \langle(\hat{p}-\bar{p})^2\rangle(t), \tag{248}$$

with $\Delta x(t) > 0$ and $\Delta p(t) > 0$. Heisenberg's uncertainty relation in this case states that one always has

$$\Delta x\, \Delta p \geq \frac{1}{2}\hbar, \tag{249}$$

for whatever quantum state $|\psi,t\rangle$, the inequality being saturated only for specific types of states. This inequality is in direct relation with the Heisenberg commutator $[\hat{q},\hat{p}] = i\hbar$. Thus any other pair of canonically conjugated observables with the same commutation relation will also obey that uncertainty relation, which may also be extended into a more general form given any commutator. As a consequence in the context of quantum physics canonically conjugated variables may no longer be known both to arbitrarily good precision, the product of the intrinsic uncertainties inherent to their quantum noncommutativity being bounded below essentially by Planck's constant.

4.3.2 The nonrelativistic quantum particle

Let us apply the previous general discussion now to the nonrelativistic particle of mass m subjected to conservative forces of total potential energy $V(\vec{r})$, of which the Lagrange function is

$$L = \frac{1}{2} m \dot{\vec{r}}^2 \, - \, V(\vec{r}) \tag{250}$$

(a generalisation to an arbitrary number of distinct particles is straightforward). The Hamiltonian of the system is

$$H = \frac{1}{2m} \vec{p}^2 \, + \, V(\vec{r}), \tag{251}$$

with the canonical phase space variables $(\vec{r}, \vec{p}) = (x^i, p_j)$ $(i, j = 1, 2, 3)$ of which the Poisson brackets are $\{x^i, p_j\} = \delta^i_j$.

Hence at the quantum level we simply have the Heisenberg algebra

$$\left[\hat{x}^i, \hat{p}_j\right] = i\hbar \, \delta^i_j, \qquad \left(\hat{x}^i\right)^\dagger = \hat{x}^i, \quad (\hat{p}_i)^\dagger = \hat{p}_i, \tag{252}$$

as well as the quantum Hamiltonian

$$\hat{H} = \frac{1}{2m} \hat{\vec{p}}^2 \, + \, V(\hat{\vec{r}}), \tag{253}$$

which is in direct correspondence with the classical Hamiltonian and is obviously also self-adjoint if the position and momentum operators are themselves self-adjoint, $\hat{H}^\dagger = \hat{H}$.

The Hilbert space of this system is simply the 3-fold tensor product of the Hilbert space of the single degree of freedom Heisenberg algebra constructed above. Diagonalisation of the Hamiltonian over that space depends on the choice of the potential energy, namely the forces to which the particle is subjected. In the case of harmonic forces for which $V(\vec{r})$ is some given but otherwise arbitrary positive definite quadratic polynomial of the cartesian coordinates x^i, a purely algebraic solution in terms of the Fock space representation of the Heisenberg algebra is readily established. However in a general case for which algebraic methods are not available, one approach to solving the eigenvalue problem is by considering the Schrödinger equation of wave quantum mechanics. Namely, consider the abstract Schrödinger equation in the Schrödinger picture,

$$\hat{H} \, |\psi, t\rangle \, = \, i\hbar \, \frac{d|\psi, t\rangle}{dt}, \tag{254}$$

and project it onto the configuration space eigenstates, leading to the Schrödinger equation for the configuration space wave function, $\psi(t, \vec{r}) = \langle \vec{r} | \psi, t \rangle$, of the quantum particle,

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 \, + \, V(\vec{r}) \right] \, \psi(t, \vec{r}) = i\hbar \, \frac{\partial \psi(t, \vec{r})}{\partial t}, \tag{255}$$

in which the correspondences $\hat{\vec{r}} \to \vec{r}$ and $\hat{\vec{p}} \to -i\hbar \vec{\nabla}$ have been applied. For a given potential energy this differential equation lends itself to methods of a more analytical or even numerical character. Note that by considering an expansion of the general state into the energy eigenbasis of which the spectrum is to be found and which may include components which are both discrete and continuous (such as the spectrum of the hydrogen atom with its discrete but yet infinite bound state spectrum and its infinite continuous spectrum of scattering or unbound states), as was done in the Fock basis in the case of the one dimensional harmonic oscillator, it suffices in fact to consider the energy eigenvalue problem for the Schrödinger equation, namely the so-called stationary Schrödinger equation,

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^{\, 2} \, + \, V(\vec{r}) \right] \, \psi_E(\vec{r}) = E \, \psi_E(\vec{r}). \tag{256}$$

Corresponding to any of the eigenvalues E of this differential eigenvalue problem, the solution to the original Schrödinger equation is then, up to an arbitrary constant phase factor both in time and space,

$$\psi_E(t, \vec{r}) = \psi_E(\vec{r}) \, e^{-\frac{i}{\hbar} E \, (t - t_0)}, \tag{257}$$

showing that this state is indeed stationary since its only time dependence is through a simple phase factor linear in time and with as coefficient the energy measured in units of $\hbar$, namely an angular frequency. The general solution to the full original Schrödinger equation is then constructed through the most general possible linear combination of all stationary states. Indeed given the energy eigenspectrum of the abstract Hamiltonian operator, $\hat{H}|E_m\rangle = E_m|E_m\rangle$, we had established in the general case that the general solution to the abstract Schrödinger equation in the Schrödinger picture is of the form,

$$|\psi, t\rangle = \sum_m |E_m\rangle\, e^{-\frac{i}{\hbar}(t-t_0)E_m}\, \langle E_m|\psi, t_0\rangle. \tag{258}$$

It suffices to project this relation onto the position eigenstates $|\vec{r}\rangle$ to obtain the same statement in terms of the configuration space wave function of the general quantum state of the system,

$$\psi(t, \vec{r}\,) = \langle \vec{r}\,|\psi, t\rangle = \sum_m \psi_{E_m}(\vec{r}\,)\, e^{-\frac{i}{\hbar}E_m(t-t_0)}\, \langle E_m|\psi, t_0\rangle. \tag{259}$$

Remark

It is also possible to write the Schrödinger equation in the Schrödinger picture in the momentum space wave function representation of the Heisenberg algebra. It should be quite clear that this equation reads,

$$\left[\frac{1}{2m}\vec{p}^{\,2} + V\left(i\hbar\vec{\nabla}\right)\right]\, \widetilde{\psi}(t, \vec{p}\,) = i\hbar\frac{\partial\widetilde{\psi}(t, \vec{r}\,)}{\partial t}. \tag{260}$$

Depending on the considered system and the issues to be solved, one of these different representations of the same abstract Schrödinger equation may be more convenient to use than the others.

Application: **The free nonrelativistic particle**

In the case of the free particle the potential energy is vanishing (or an arbitrary constant, leading to an arbitrary constant phase redefinition of the quantum states). It is best to consider the Schrödinger equation (in the Schrödinger picture) in the momentum representation since it is obvious that the energy eigenstates are then simply the momentum eigenstates, $|\vec{p}\rangle$, with

$$\hat{H}\,|\vec{p}\rangle = E(\vec{p}\,)\,|\vec{p}\rangle, \qquad E(\vec{p}\,) = \frac{1}{2m}\vec{p}^{\,2}. \tag{261}$$

Consequently the stationary solutions to the configuration space Schrödinger equation are

$$\psi_{\vec{p}}(t, \vec{r}\,) = \langle \vec{r}\,|\vec{p}, t\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\, e^{\frac{i}{\hbar}\vec{r}\cdot\vec{p}}\, e^{-\frac{i}{\hbar}(t-t_0)\,E(\vec{p}\,)}. \tag{262}$$

It is also possible to consider the Schrödinger equation in the Heisenberg picture. It should be quite clear that the solution to that equation in the case of the position and momentum operators is of the form

$$\hat{\vec{r}}(t) = \hat{\vec{r}}(t_0) + \frac{1}{m}\hat{\vec{p}}(t_0)\,(t - t_0), \qquad \hat{\vec{p}}(t) = \hat{\vec{p}}(t_0), \tag{263}$$

which are indeed the operator solutions in direct correspondence with their classical counterparts in the Hamiltonian formulation of the same system. Once again we notice that when the full quantum dynamics may be solved, the Heisenberg picture of that dynamics is in direct correspondence with the classical solutions to the Hamiltonian first order equations of motion for the observables.

4.3.3 The one dimensional harmonic oscillator

In the case of this system the configuration space Schrödinger equation (in the Schrödinger picture) reads, given the potential energy $V(q) = m\omega^2 q^2/2$,

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}m\omega^2 q^2\right]\, \psi(t, q) = i\hbar\frac{\partial\psi(t, q)}{\partial t}. \tag{264}$$

Even the Schrödinger equation for stationary states,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{1}{2}m\omega^2 q^2\right]\psi_n(q) = E_n\,\psi_n(q), \tag{265}$$

where an index n distinguishing energy eigenvalues has already been introduced, is not the most appealing. Solving this differential eigenvalue problem is not readily achieved, and has produced historically a certain class of special functions, namely the Hermite polynomials.

However, let us show how the knowledge of the purely algebraic solution based on Fock space techniques allows a direct resolution of the above differential equation. First, we already know that the spectrum of energy eigenvalues is given by

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \qquad n = 0, 1, 2, \ldots \tag{266}$$

To each of these eigenvalues there thus corresponds an eigen-wave function $\psi_n(q) = \langle q|n\rangle$ for the associated stationary state $\psi_n(t,q) = e^{-\frac{i}{\hbar}(t-t_0)E_n}\,\psi_n(q)$, which is nothing else but the configuration space wave function of the Fock state $|n\rangle$. In other words, solving the problem of determining these eigenfunctions $\psi_n(q)$ amounts also to establishing the change of basis between the Fock basis of the abstract Hilbert space providing the representation (up to unitary equivalence) and the configuration space basis of the position eigenstates $|q\rangle$.

In order to identify the functions $\psi_n(q)$, let us return to the defining property of the Fock states, beginning with the Fock vacuum which is annihilated by the operator a, $a|0\rangle = 0$. Hence, projecting that relation onto a position eigenstate $|q\rangle$, we have

$$\langle q|a|0\rangle = 0. \tag{267}$$

However, in terms of the abstract operators we have

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{q} + \frac{i}{m\omega}\hat{p}\right], \tag{268}$$

so that when acting on configuration space wave functions the abstract operator a is realised by the functional operator

$$a: \qquad \sqrt{\frac{m\omega}{2\hbar}}\left[q + \frac{\hbar}{m\omega}\frac{d}{dq}\right]. \tag{269}$$

Consequently the above property for the Fock vacuum, $\langle q|a|0\rangle = 0$, translates into the following differential equation for the configuration space wave function of the ground state, $\psi_0(q) = \langle q|0\rangle$,

$$\left[q + \frac{\hbar}{m\omega}\frac{d}{dq}\right]\psi_0(q) = 0, \tag{270}$$

of which the solution is

$$\psi_0(q) = N\,e^{-\frac{m\omega}{2\hbar}q^2}, \tag{271}$$

N being some complex normalisation constant. The latter is fixed by the normalisation condition of the Fock vacuum,

$$1 = \langle 0|0\rangle = \int_{-\infty}^{+\infty} dq\,\langle 0|q\rangle\,\langle q|0\rangle = \int_{-\infty}^{+\infty} dq\,|\langle q|0\rangle|^2 = |N|^2\int_{-\infty}^{+\infty} dq\,e^{-\frac{m\omega}{\hbar}q^2} = |N|^2\sqrt{\frac{\pi\hbar}{m\omega}}. \tag{272}$$

Hence, up to an arbitrary choice of phase set to unity once again (*i.e.*, up a unitary transformation in Hilbert space), one has finally the configuration space wave function of the Fock vacuum,

$$\psi_0(q) = \langle q|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}q^2}. \tag{273}$$

In order to also determine the wave functions for the excited Fock states,

$$\psi_n(q) = \langle q|n\rangle = \frac{1}{\sqrt{n!}}\,\langle q|\left(a^\dagger\right)^n|0\rangle, \tag{274}$$

we now need to consider the functional operator realisation of the abstract creation operator, $a^\dagger$, in the configuration space representation of the Heisenberg algebra. From the above discussion in the case of the annihilation operator a, it is clear that we have the correspondence,

$$a^\dagger : \qquad \sqrt{\frac{m\omega}{2\hbar}} \left[q - \frac{\hbar}{m\omega} \frac{d}{dq} \right]. \tag{275}$$

Consequently,

$$\psi_n(q) = \frac{1}{\sqrt{n!}} \left(\frac{m\omega}{2\hbar} \right)^{n/2} \left[q - \frac{\hbar}{m\omega} \frac{d}{dq} \right]^n \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar} q^2}, \tag{276}$$

in which the function $\psi_0(q) = \langle q|0\rangle$ has already been substituted by its solution established previously. This expression is reminiscent of one possible definition of the Hermite polynomials, namely

$$H_n(x) = e^{\frac{1}{2}x^2} \left[x - \frac{d}{dx} \right]^n e^{-\frac{1}{2}x^2}, \quad n = 0, 1, 2, \ldots \tag{277}$$

Hence, by an appropriate rescaling of the coordinate q, the above expression for $\psi_n(q)$ may be brought into the form of this definition of the Hermite polynomials. All factors combine to give the following final expression for the configuration space wave functions of the energy eigenstates of the harmonic oscillator,

$$\psi_n(q) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{\sqrt{2^n\, n!}} e^{-\frac{m\omega}{2\hbar} q^2} H_n \left(q \sqrt{\frac{m\omega}{\hbar}} \right). \tag{278}$$

As indicated already previously in the general case, from the knowledge of these stationary solutions one may construct the expression for the general solution to the Schrödinger equation (in the Schrödinger picture) in the configuration space representation of the Heisenberg algebra. Incidentally, since the Hamiltonian is quadratic in both p and q, the solution in the momentum space wave function representation is again constructed in terms of the Hermite polynomials evaluated for a rescaling of the conjugate momentum variable p. The Fourier transformation of the above products of the Hermite polynomials with the Gaussian factor included produces again similar products of the same Hermite polynomial with a common Gaussian factor, but of course now as a function of p rather than q including some appropriate dimensionful scaling parameters as displayed for instance in the above explicit expression for the configuration space solutions.

4.4 The path integral representation and quantisation

It is well known that besides the canonical quantisation path, there is another royal avenue towards the quantisation of a classical system whose dynamics is defined through some action and the variational principle, namely the so-called path integral or functional integral formulation of quantum mechanics. Here we shall discuss how, starting from the canonical quantisation of any such system following the approach outlined in the previous Sections, it is possible to set up integral representations for matrix elements of quantum operators, which acquire the interpretation of functional integrals over phase space. When reducing from these integrals the conjugate momentum degrees of freedom, one recovers a functional integral over configuration space in which the original classical action expressed in terms of the Lagrange function plays again a central rôle. Further remarks as to quantisation directly through the functional integral are made at the end of this discussion. It should already be clear that these two approaches are complementary, each with its own advantages and difficulties both with respect to an intuitive understanding of the physics that they both encode as well as to the calculational advantages of one compared to the other. However, when properly implemented, they represent in complementary ways an identical physical content.

The procedure for constructing an integral representation for matrix elements of operators, starting from canonical quantisation, follows essentially always the same avenue, based on the insertion of complete sets of states in terms of which the unit operator possess a spectral resolution. Here, we shall illustrate this feature for the configuration and momentum space representations of the Heisenberg algebra, even though more general cases may be envisaged as well. In a later Section such an illustration will be provided in terms of so-called coherent states, to be introduced hereafter. Furthermore, we shall consider configuration space matrix elements of the evolution operator for a given quantum system, namely the

propagator $\langle q_f|U(t_f,t_i)|q_i\rangle$ of the system (in configuration space[12]). Indeed, the physical meaning of this quantity is that it measures the overlap with the position eigenstate $|q_f\rangle$ of the time evolved position eigenstate $|q_i\rangle$ over the time interval $(t_f - t_i)$, namely the probability amplitude for finding the system, initially localised at $q = q_i$ at time $t = t_i$, at the position $q = q_f$ at time $t = t_f$: this is indeed the probability amplitude for propagating the system in configuration space for a given time interval.

The quantum evolution operator may also be expressed as the product of such operators representing the evolution of the system through a succession of time slices,

$$U(t_f,t_i) = e^{-\frac{i}{\hbar}(t_f-t_i)\hat{H}} = \left[e^{-\frac{i}{\hbar}\epsilon\hat{H}}\right]^N = \lim_{N\to\infty}\left[1-\frac{i}{\hbar}\epsilon\hat{H}\right]^N, \tag{279}$$

with

$$\epsilon = \frac{t_f-t_i}{N} = \frac{\Delta t}{N}, \qquad \Delta t = t_f - t_i, \tag{280}$$

while N is some arbitrary positive integer specifying an equally spaced slicing of the finite time interval $(t_f - t_i)$. In what follows, the n index for the degrees of freedom (q^n, p_n) is suppressed, to keep expressions as transparent as possible. Given this time sliced form of the evolution operator, the idea now is to insert twice the spectral resolution of the unit operator $\mathbb{I}$, once in terms of the position eigenstates, and once in terms of the momentum eigenstates, and this in between each of the N factors that appear in the above N factorised form for $U(t_f,t_i)$, as follows,

$$\mathbb{I} = \int_{-\infty}^{+\infty} dp_\alpha \int_{-\infty}^{+\infty} dq_{\alpha+1}\, |q_{\alpha+1}\rangle\langle q_{\alpha+1}|p_\alpha\rangle\langle p_\alpha|, \qquad \alpha = 0,1,2,\ldots,N-2. \tag{281}$$

Setting then $q_f = q_{\alpha=N}$ and $q_i = q_{\alpha=0}$, a straightforward substitution into the considered matrix element leads to the expression (a substitution of the unit operator as $\mathbb{I} = \int_{-\infty}^{+\infty} dp|p\rangle\langle p|$ is also performed to the right of the external final state $\langle q_f|$, leading to one more integration over the p_α's than over the q_α's),

$$\langle q_f|U(t_f,t_i)|q_i\rangle = \int_{-\infty}^{+\infty}\prod_{\alpha=1}^{N-1} dq_\alpha \prod_{\alpha=0}^{N-1} dp_\alpha \prod_{\alpha=0}^{N-1}\left[\langle q_{\alpha+1}|p_\alpha\rangle\langle p_\alpha|e^{-\frac{i}{\hbar}\epsilon\hat{H}}|q_\alpha\rangle\right]. \tag{282}$$

Using then the value for the matrix element $\langle q|p\rangle$ given previously, this quantity finally reduces to,

$$\langle q_f|U(t_f,t_i)|q_i\rangle = \lim_{N\to\infty}\int_{-\infty}^{+\infty}\prod_{\alpha=1}^{N-1} dq_\alpha \prod_{\alpha=0}^{N-1}\frac{dp_\alpha}{2\pi\hbar}\exp\left\{\frac{i}{\hbar}\sum_{\alpha=0}^{N-1}\epsilon\left[\frac{q_{\alpha+1}-q_\alpha}{\epsilon}p_\alpha - h_\alpha\right]\right\}, \tag{283}$$

with the Hamiltonian matrix elements

$$h_\alpha = \frac{\langle p_\alpha|\hat{H}|q_\alpha\rangle}{\langle p_\alpha|q_\alpha\rangle}. \tag{284}$$

Clearly, the discretised integral representation (283) of the configuration space propagator corresponds to a specific construction of the otherwise formal expression for the phase space path integral or functional integral corresponding to that quantity, namely the following integral over the space of functions $q(t)$ and $p(t)$,

$$\langle q_f|U(t_f,t_i)|q_i\rangle = \int_{q(t_i)=q_i}^{q(t_f)=q_f}\left[\mathcal{D}q\frac{\mathcal{D}p}{2\pi\hbar}\right] e^{\frac{i}{\hbar}S[q,p]}, \tag{285}$$

in which the phase space action is that of the first-order Hamiltonian formulation of the system, namely

$$S[q,p] = \int_{t_i}^{t_f} dt\,[\dot{q}p - H(q,p)], \tag{286}$$

which is that associated to the choice of boundary conditions corresponding to the configuration space propagator when imposing the variational principle in a strong sense, namely with the induced boundary terms also required to vanish through the boundary conditions $q(t_{i,f}) = q_{i,f}$. Note that contrary to

[12]It would be an excellent exercise to establish a path integral representation for the momentum space matrix elements of the same operator.

what the formal expression (285) may lead one to believe, the integration measure is not quite the phase space Liouville measure, since in fact there is always one more p_α integration than the number of q_α integrations. One should always keep this remark in mind when developing formal arguments based on the formal expression (285) of the functional integral.

Considering the momentum space matrix elements of the same operator, a similar analysis leads to an analogous specific discretised expression, namely

$$\langle p_f|U(t_f,t_i)|p_i\rangle = \lim_{N\to\infty}\int_{-\infty}^{+\infty}\prod_{\alpha=1}^{N-1}dp_\alpha\prod_{\alpha=0}^{N-1}\frac{dq_\alpha}{2\pi\hbar}\exp\left\{\frac{i}{\hbar}\sum_{\alpha=0}^{N-1}\epsilon\left[-q_\alpha\frac{p_{\alpha+1}-p_\alpha}{\epsilon}-h_\alpha\right]\right\}, \tag{287}$$

with $h_\alpha = \langle q_\alpha|\hat{H}|p_\alpha\rangle/\langle q_\alpha|p_\alpha\rangle$, corresponding to the formal quantity,

$$\langle p_f|U(t_f,t_i)|p_i\rangle = \int_{p(t_i)=p_i}^{p(t_f)=p_f}\left[\frac{\mathcal{D}q}{2\pi\hbar}\mathcal{D}p\right]\, e^{\frac{i}{\hbar}S[q,p]}, \tag{288}$$

where the appropriate Hamiltonian first-order action now reads

$$S[q,p] = \int_{t_i}^{t_f} dt\,[-q\dot{p}-H(q,p)]\,, \tag{289}$$

being this time associated to the choice of boundary conditions $p(t_{i,f}) = p_{i,f}$ as opposed to $q(t_{i,f}) = q_{i,f}$ for the propagator in configuration space. Note that the same remark as above concerning the phase space Liouville measure applies here as well.

In the particular situation that the Hamiltonian is such that the matrix elements h_α are quadratic in the momenta,

$$h_\alpha = \frac{p_\alpha^2}{2m}+V(q_\alpha), \tag{290}$$

which is the case when the quantum Hamiltonian is of the form $\hat{H} = \hat{p}^2/2m + V(\hat{q})$, the integration over momentum space may be completed explicitly in the above discretised expressions[13], thereby leading to the configuration space functional integral representation,

$$\langle q_f|U(t_f,t_i)|q_i\rangle = \lim_{N\to\infty}\left(\frac{m}{2i\pi\hbar\epsilon}\right)^{N/2}\int_{-\infty}^{+\infty}\prod_{\alpha=1}^{N-1}dq_\alpha\exp\left\{\frac{i}{\hbar}\sum_{\alpha=0}^{N-1}\epsilon\left[\frac{1}{2}m\left(\frac{q_{\alpha+1}-q_\alpha}{\epsilon}\right)^2-V(q_\alpha)\right]\right\}, \tag{291}$$

or at the formal level,

$$\langle q_f|U(t_f,t_i)|q_i\rangle = \int_{q(t_i)=q_i}^{q(t_f)=q_f}[\mathcal{D}q]\; e^{\frac{i}{\hbar}S[q]}, \tag{292}$$

with

$$S[q] = \int_{t_i}^{t_f} dt\, L(q,\dot{q}), \qquad L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q). \tag{293}$$

The above explicit discretised representation of this latter formal functional integral coincides exactly with the explicit construction performed by Feynman when he first developed the path integral quantisation approach [7].

Hence, we have come back full circle. Starting from the action principle defined within the Lagrangian formulation of dynamics, the canonical Hamiltonian formulation of the same dynamics on phase space has been constructed, allowing for the canonical operator quantisation of the associated algebraic and geometric structures, for which operator matrix elements may be given a functional integral representation on phase space or configuration space, in which the classical Hamiltonian or Lagrangian action functionals reappear on equal terms. The concept which is central to this whole construction is that of the action, through one of the many forms by which it contributes whether for the classical or the quantum dynamics.

[13] Using the following Gaussian integral, $\int_{-\infty}^{+\infty} dx e^{-\alpha x^2} = \sqrt{\pi/\alpha}$, valid within the complex plane through analytic continuation from the region with $\mathrm{Re}\,\alpha > 0$.

Having chosen to follow the operator quantisation path, once a specific choice of operator ordering has been made, in principle the functional integral representation acquires a totally unambiguous and well defined discretised expression, which defines in an exact manner otherwise ill defined formal path integral expressions whose actual meaning always still needs to be specified properly. Nonetheless, as we have indicated, difficulties lie at the operator level precisely in the choice of operator ordering required so as to obtain a consistent unitary quantum theory.

Had one taken the functional integral path towards quantisation, whether from the Lagrangian or Hamiltonian classical actions, the difficulty of a proper construction of the quantised system then lies hidden in the necessity of giving a precise definition and meaning, through some discretisation procedure or otherwise, to the formal and thus ill defined functional integrals such as those in (285), (288) and (292). As a matter of fact, the arbitrariness which exists at this level in the choice of discretisation procedure and functional integration measure (whether over configuration, momentum or phase space) is in direct correspondence with the arbitrariness which exists on the operator side of this relationship in terms of the choice of operator ordering. Taking either path towards quantisation, for appropriate choices on both sides which are in correspondence, the same dynamical quantum system is being represented in a complementary manner. It is extremely fruitful to constantly keep in one's mind these equivalent representations of a quantum dynamics when properly implemented, in particular in a manner that should ensure its quantum unitarity.

As a final illustration, consider the free nonrelativistic particle, with $V(q) = 0$. Given the exact expression in (291), the remaining Gaussian integrations may then all be completed, leading *in fine* to the matrix element,

$$\langle q_f|U(t_f,t_i)|q_i\rangle = \Big(\frac{m}{2i\pi\hbar\Delta t}\Big)^{1/2}\, e^{\frac{i}{\hbar}\frac{m}{2\Delta t}(q_f-q_i)^2} = \Big(\frac{m}{2i\pi\hbar\Delta t}\Big)^{1/2}\, e^{\frac{i}{\hbar}S_c}, \tag{294}$$

with for the classical action S_c,

$$q(t) = q_i + \frac{q_f-q_i}{\Delta t}(t-t_i), \quad \dot q(t) = \frac{q_f-q_i}{\Delta t}, \quad S_c = \int_{t_i}^{t_f} dt\, \frac{1}{2}m\dot q^2 = \frac{m}{2\Delta t}\,(q_f-q_i)^2\,. \tag{295}$$

As a matter of fact, that the classical action appears as a phase factor in the overall path integral and this matrix element is no accident, but may be understood through a saddle point evaluation of the path integral[14] which happens to be exact in the present case, and more generally for any Lagrange function which is quadratic in q and $\dot q$, as is also the case for the harmonic oscillator. That the above expression for this matrix element is correct may also be checked directly from the wave function representations of the Heisenberg algebra, and using the momentum representation in which the Hamiltonian, hence the quantum evolution operator $U(t_f,t_i)$, is diagonal. This is left as a useful exercise to the reader.

A few more remarks are in order. First, it is straightforward to extend to an arbitrary number N of degrees of freedom (q^n,p_n) both the above discretised and the formal expressions for the relevant path integral representations of matrix elements. Second, by proper consideration of representations of the Heisenberg algebra on an arbitrary configuration space[15], possibly with nontrivial curvature and when curvilinear coordinates are used, even in the Euclidean case, it is possible to extend the analysis to such situations as well. When configuration space possesses nontrivial topology, extra features of a purely quantum character then also come into play, having to do with the first homotopy group of the configuration manifold and its U(1) holonomy representations [6]. Finally, in spite of appearances from its formal representation, the precise construction of the path integral over phase space is not invariant under canonical transformations of phase space—which indeed leave the phase space Liouville measure invariant—, since the integration measure in the path integral is not exactly the Liouville measure.

[14]Such a saddle point evaluation is equivalent to the classical limit $\hbar \to 0$, which is such that only the classical trajectories, which extremise the classical action, end up contributing to the path integral. From that point of view, this very fact is a justification *a posteriori* for the variational principle of classical dynamics.

[15]These representations are not being discussed in these notes.

4.5 Representations of the Heisenberg algebra II: Coherent states

So far for a single degree of freedom system, we have constructed essentially three different though unitarily equivalent representations of the Heisenberg algebra,

$$[\hat{q},\hat{p}] = i\hbar, \qquad \hat{q}^\dagger = \hat{q}, \qquad \hat{p}^\dagger = \hat{p}, \tag{296}$$

namely the configuration space and momentum space wave function representations in terms of square integrable wave functions on the real line, $q, p \in \mathbb{R}$, and in terms of the Fock algebra associated to the Heisenberg algebra provided a parameter with the physical dimensions of $(m\omega)$ is available, as is the case for the harmonic oscillator. Once the Fock space representation is achieved, it is possible to identify yet another realisation of the Heisenberg algebra, in terms of so-called canonical coherent states. The notion of coherent state extends much beyond the simple Heisenberg algebra, but retains most of the properties of the canonical coherent states discussed hereafter. Note also that the discussion will be restricted to a single degree of freedom, but may readily be extended to many degrees of freedom through a simple tensor product of Hilbert spaces.

In order to identify a Fock algebra associated to the above Heisenberg algebra, one needs to introduce an extra real and positive parameter, to be denoted $\lambda > 0$ hereafter, having the physical dimensions of a mass multiplying an angular frequency (after all, this is the situation for the harmonic oscillator, but here the discussion does not presume a specific dynamics; it remains of a purely kinematical character). Given such a parameter, consider then the operators,

$$a = \sqrt{\frac{\lambda}{2\hbar}}\left[\hat{q} + \frac{i}{\lambda}\hat{p}\right], \qquad a^\dagger = \sqrt{\frac{\lambda}{2\hbar}}\left[\hat{q} - \frac{i}{\lambda}\hat{p}\right], \tag{297}$$

and their inverse relations,

$$\hat{q} = \sqrt{\frac{\hbar}{2\lambda}}\left[a + a^\dagger\right], \qquad \hat{p} = -i\lambda\sqrt{\frac{\hbar}{2\lambda}}\left[a - a^\dagger\right]. \tag{298}$$

It is clear that the operators $(a, a^\dagger)$ span a Fock algebra over the Hilbert space associated to the original Heisenberg algebra,

$$\left[a, a^\dagger\right] = \mathbb{I}. \tag{299}$$

Consequently, the associated Fock states span a discrete basis of this Hilbert space. Consider the Fock vacuum state $|\Omega\rangle$ associated to the choice of λ, defined by the properties

$$a|\Omega\rangle = 0, \qquad \langle\Omega|\Omega\rangle = 1, \tag{300}$$

as well as the Fock states $|n\rangle$ $(n = 0, 1, 2, \ldots)$,

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n |\Omega\rangle, \qquad \langle n|m\rangle = \delta_{n,m}, \qquad \mathbb{I} = \sum_{n=0}^{+\infty} |n\rangle\langle n|. \tag{301}$$

As we know one has the following actions of the ladder, or creation and annihilation operators,

$$a|n\rangle = \sqrt{n}\,|n-1\rangle, \qquad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle, \qquad N = a^\dagger a: \quad N|n\rangle = n\,|n\rangle. \tag{302}$$

In particular

$$|\psi\rangle = \sum_{n=0}^{+\infty} |n\rangle\,\psi_n, \qquad \psi_n = \langle n|\psi\rangle, \tag{303}$$

while the change of basis from the Fock state basis to the configuration space eigenbasis, say, is specified by the matrix elements

$$\langle q|n\rangle = \left(\frac{\lambda}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}\, e^{-\frac{\lambda}{2\hbar}q^2}\, H_n\left(q\sqrt{\frac{\lambda}{\hbar}}\right), \tag{304}$$

$H_n(x)$ being the Hermite polynomials of order $n \in \mathbb{N}$. These functions thus provide a complete and infinite discrete basis in $L^2(\mathbb{R}, dx)$.

Remark

It is of interest to consider this discussion in the specific case of the harmonic oscillator once again, with

$$L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2, \qquad H(q,p) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2. \tag{305}$$

At the quantum level one then finds

$$\begin{aligned} \hat{H} &= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{q}^2 \\ &= \frac{\hbar}{2m\lambda}\left[(m\omega)^2 + \lambda^2\right]\left[a^\dagger a + \frac{1}{2}\right] + \frac{\hbar}{4m\lambda}\left[(m\omega)^2 - \lambda^2\right]\left[{a^\dagger}^2 + a^2\right]. \end{aligned} \tag{306}$$

Hence the choice of Fock algebra which diagonalises the Hamiltonian of the system corresponds to the value $\lambda = m\omega$, readily leading to the energy spectrum,

$$\hat{H} = \hbar\omega\left[a^\dagger a + \frac{1}{2}\right], \qquad \hat{H}|n\rangle = E_n\,|n\rangle, \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right). \tag{307}$$

4.5.1 Phase space or canonical coherent states

Given the Fock algebra constructed as indicated above, the associated phase space or canonical coherent states are defined according to the following relations. Given any point (q,p) in phase space, namely any classical state, there corresponds to it a quantum state in Hilbert space parametrised by these two coordinates and obtained from the exponentiated action of the Heisenberg algebra, or the Fock algebra, on the Fock vacuum[16], $|\Omega\rangle$,

$$|q,p\rangle = e^{-\frac{i}{\hbar}(q\hat{p}-p\hat{q})}\,|\Omega\rangle = e^{-\frac{1}{2}|z|^2}\,e^{za^\dagger}\,|\Omega\rangle = |z\rangle, \qquad |z\rangle = e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{+\infty}\frac{z^n}{\sqrt{n!}}\,|n\rangle, \tag{308}$$

with

$$z = \sqrt{\frac{\lambda}{2\hbar}}\left[q + \frac{i}{\lambda}p\right], \qquad \bar{z} = \sqrt{\frac{\lambda}{2\hbar}}\left[q - \frac{i}{\lambda}p\right]. \tag{309}$$

Note how this complex parameter labelling phase space is in direct correspondence with the relations defining the creation and annihilation operators in terms of the position and momentum operators $\hat{q}$ and $\hat{p}$. It is the very last relation on the r.h.s. of (308) which explains the name given to these states. Indeed, each of the Fock quantum states $|n\rangle$ are involved but with relative phases for the coefficients which define their combination which are coherent, namely given by the successive powers of the unique and common complex parameter z. In fact, coherent states play a central rôle in quantum optics, for instance, or any other field where coherence effects are at play, as is the case for laser physics and the optical coherence properties of laser beams. Coherent states also play an important rôle in quantum field theory, as models for the quantum states corresponding to classical fields, such as classical electric and magnetic fields.

The different expressions above for these coherent states follow from applying the following Baker–Campbell–Hausdorff formula valid for any two operators A and B,

$$e^A\,e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]-\frac{1}{12}[B,[A,B]]+\cdots}. \tag{310}$$

In particular if $[A,B]$ commutes with both A and B, this formula reduces to

$$e^{A+B} = e^{-\frac{1}{2}[A,B]}\,e^A\,e^B, \tag{311}$$

which is the relevant situation in the present case.

A first noteworthy property of these coherent states is that they are eigenstates of the annihilation operator,

$$a|z\rangle = z\,|z\rangle, \quad a^n|z\rangle = z^n\,|z\rangle. \tag{312}$$

[16] In fact, most properties characteristic of coherent states discussed hereafter remain applicable whatever the choice of normalised "fiducial" quantum state chosen in place of $|\Omega\rangle$.

Also, the overlap of any such coherent state with a Fock state is a pure monomial in z, except for a common Gaussian factor,

$$\langle n|z\rangle = \frac{1}{\sqrt{n!}}\langle\Omega|a^n|z\rangle = \frac{1}{\sqrt{n!}}\, e^{-\frac{1}{2}|z|^2}\, z^n. \tag{313}$$

Since it will turn out that coherent states define yet another (overcomplete) basis of Hilbert space, this fact shows that in that basis Fock states are represented by simple monomials in z, as compared to Hermite polynomials in configuration (or momentum) space, a much welcome simpler situation.

Even though the above coherent states are normalised, $\langle z|z\rangle = 1$, their general overlaps are nonvanishing,

$$\langle z_1|z_2\rangle = e^{-\frac{1}{2}|z_1|^2-\frac{1}{2}|z_2|^2+\bar{z}_1 z_2}, \qquad \langle z|z\rangle = 1, \qquad \langle z_1|z_2\rangle \neq 0, \tag{314}$$

or in terms of the real (q,p) parametrisation,

$$\langle q_2,p_2|q_1,p_1\rangle = \exp\left\{-\frac{\lambda}{4\hbar}\left[(q_2-q_1)^2+\frac{1}{\lambda^2}\,(p_2-p_1)^2\right] + \frac{i}{2\hbar}\,(q_2p_1-q_1p_2)\right\}. \tag{315}$$

Hence even though coherent states span the entire Hilbert space they are not linearly independent, namely they provide an overcomplete basis of the space of states. The fact that they generate the whole space of quantum states follows from the **overcompleteness relation**, or resolution of the unit operator in terms of coherent states.

$$\mathbb{I} = \int_{\mathbb{R}^2} \frac{dqdp}{2\pi\hbar}\, |q,p\rangle\,\langle q,p| = \int_{\mathbb{C}} \frac{dzd\bar{z}}{\pi}\, |z\rangle\,\langle z| \qquad [dzd\bar{z} = d\mathrm{Re}\, z\, d\mathrm{Im}\, z]. \tag{316}$$

This relation may be verified by computing explicitly all its matrix elements in the Fock state basis, for instance. Indeed, this resolution of the unit operator is a nontrivial property of coherent states which is crucial for the relevance of these states to quantum physics in general.

Given the resolution of the unit operator in terms of coherent states, and as was the case for the configuration and momentum space wave function representations of quantum states, coherent states lead to (anti)holomorphic (also called Bargmann) wave function representations of quantum states, namely in terms of functions of the variable $\bar{z}$ only, again up to an overall and common Gaussian factor $\exp(-|z|^2/2)$,

$$\psi(z) = \langle z|\psi\rangle = e^{-\frac{1}{2}|z|^2}\,\varphi(\bar{z}), \qquad |\psi\rangle = \int_{\mathbb{C}} \frac{dzd\bar{z}}{\pi}\, |z\rangle\,\psi(z) = \int_{\mathbb{C}} \frac{dzd\bar{z}}{\pi}\, e^{-\frac{1}{2}|z|^2}\, |z\rangle\,\varphi(\bar{z}). \tag{317}$$

Consequently, one has the following representations for the annihilation and creation operators,

$$\begin{aligned} a: \quad \langle z|a|\psi\rangle &= \left[\partial_{\bar{z}} + \frac{1}{2}z\right]\,\psi(z) = e^{-\frac{1}{2}|z|^2}\,\partial_{\bar{z}}\varphi(\bar{z}), \\ a^\dagger: \quad \langle z|a^\dagger|\psi\rangle &= \bar{z}\,\psi(z) = e^{-\frac{1}{2}|z|^2}\,\bar{z}\,\varphi(\bar{z}). \end{aligned} \tag{318}$$

Coherent states still possess other noteworthy properties. For instance the diagonal matrix elements for both $\hat{q}$ and $\hat{p}$ are both sharp in phase space,

$$\bar{q} = \langle q,p|\hat{q}|q,p\rangle = q, \qquad \bar{p} = \langle q,p|\hat{p}|q,p\rangle = p. \tag{319}$$

In view of Heisenberg's uncertainty principle, such a property is remarkable indeed. It needs to be emphasized though, that it is true only provided the diagonal matrix elements in the coherent state basis are considered; non diagonal matrix elements of these same two operators do not possess that property. Nevertheless, when considering the Heisenberg uncertainty relation itself for any coherent state $|z\rangle$, one in fact finds that this relation is exactly saturated whatever the value for z,

$$(\Delta q)^2 = \langle q,p|\,(\hat{q}-\bar{q})^2\,|q,p\rangle = \frac{\hbar}{2\lambda} \quad , \quad (\Delta p)^2 = \langle q,p|\,(\hat{p}-\bar{p})^2\,|q,p\rangle = \frac{1}{2}\hbar\lambda, \tag{320}$$

$$\Delta q\,\Delta p = \frac{1}{2}\hbar. \tag{321}$$

Consequently, coherent states are quantum states which are closest to being ordinary classical states, sharing quite a number of properties of classical states, being in particular eigenstates of a with as eigenvalue z, and in one-to-one correspondence with classical states in phase space.

Yet another property characteristic of coherent states in general is that the above canonical coherent states are stable under time evolution. Consider as time evolution generating Hamiltonian the operator $\hat{H} = \hbar\omega(a^\dagger a + 1/2)$. A straightforward application of the following Baker–Campbell–Hausdorff formula,

$$e^A e^B e^{-A} = e^{B+[A,B]+\frac{1}{2!}[A,[A,B]]+\frac{1}{3!}[A,[A,[A,B]]]+\cdots}, \tag{322}$$

then finds

$$e^{-\frac{i}{\hbar}\hat{H}t}\,|z\rangle = e^{-\frac{1}{2}i\omega t}\,|ze^{-i\omega t}\rangle. \tag{323}$$

This remarkable property implies that in the case of the harmonic oscillator, given the one-to-one correspondence between classical states in classical phase space and quantum coherent states in quantum Hilbert space, the time evolution of the latter in quantum space is in one-to-one correspondence with the classical trajectory in phase space. Other dynamical systems for which coherent states may be constructed in a similar manner also share this remarkable property. The canonical coherent states discussed here are the coherent states associated to the Weyl–Heisenberg group and to the harmonic oscillator.

In fact, having established this time dependence for the coherent states of the harmonic oscillator, and using the overlap of phase space coherent states as given above, it follows that the phase space coherent state matrix elements of the quantum evolution operator of the harmonic oscillator are given by, with $\Delta t = t_f - t_i$ and of course the choice $\lambda = m\omega$,

$$\begin{aligned}\langle q_f, p_f| \quad U(t_f,t_i)|q_i,p_i\rangle &= e^{-\frac{1}{2}i\omega\Delta t}\, e^{\frac{i}{2\hbar}(q_f p_i - q_i p_f)e^{-i\omega\Delta t}} \times \\ &\times \exp\left\{-\tfrac{m\omega}{4\hbar}\left[q_f^2+q_i^2-2q_fq_ie^{-i\omega\Delta t}\right] - \tfrac{1}{4\hbar m\omega}\left[p_f^2+p_i^2-2p_fp_ie^{-i\omega\Delta t}\right]\right\}.\end{aligned} \tag{324}$$

The small time, $\Delta t \to 0$, behaviour of this quantity is thus the basic building block for the construction of a path integral representation of such phase space coherent state matrix elements, to be described hereafter.

As a final remark, let us consider an application of coherent states to diagonalise the harmonic oscillator coupled to an external dipole field leading to a shifted vacuum state,

$$L = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2q^2 - \alpha q = \frac{1}{2}m\dot{Q}^2 - \frac{1}{2}mQ^2 + \frac{\alpha^2}{2m\omega^2}, \qquad Q(t) = q(t) + \frac{\alpha}{m\omega}. \tag{325}$$

Here the variable $Q(t)$ is such that it vanishes at the minimum of the total potential energy $V(q) = m\omega^2q^2/2 + \alpha q$. In terms of the annihilation operators associated to Q (*i.e.*, A) and q (*i.e.*, a), which, given the above definition of Q in terms of q, are related as

$$A = a + \sqrt{\frac{m\omega}{2\hbar}}\frac{\alpha}{m\omega} = a + \frac{\alpha}{\sqrt{2\hbar m\omega}}, \tag{326}$$

it obviously follows that the actual ground state of the shifted oscillator is a specific coherent state of the ground state of the unshifted oscillator, when $\alpha = 0$, since one has

$$A|\Omega_\alpha\rangle = 0 \Longrightarrow a|\Omega_\alpha\rangle = -\frac{\alpha}{\sqrt{2\hbar m\omega}}|\Omega_\alpha\rangle. \tag{327}$$

Since coherent states are eigenstates of the annihilation operator a, up to an arbitrary phase factor, the unique normalised solution to the latter condition is thus given by the following coherent state,

$$|\Omega_\alpha\rangle = |z(\alpha)\rangle = e^{-\frac{1}{2}|z(\alpha)|^2}\, e^{z(\alpha)a^\dagger}\,|\Omega\rangle, \quad z(\alpha) = -\frac{\alpha}{\sqrt{2\hbar m\omega}}. \tag{328}$$

This shows that when $\alpha \neq 0$, the true vacuum of the system is the vacuum of the original system filled with a "condensate" of a coherent infinite number of quanta of the original system. When $\alpha \neq 0$, the point $q = 0$ is no longer the minimum of the potential energy but becomes unstable and decays into the true ground state at $Q = 0$, which at the quantum level corresponds to the nonperturbative coherent vacuum state $|\Omega_\alpha\rangle = |z(\alpha)\rangle$.

4.5.2 The coherent state phase space path integral

Given the resolution of the unit operator in terms of the phase space coherent states,

$$\mathbb{I} = \int_{\mathbb{R}^2} \frac{dqdp}{2\pi\hbar} \, |q,p\rangle \, \langle q,p|, \tag{329}$$

in a manner analogous to the one discussed previously for the construction of path integral representations of configuration or momentum space matrix elements of the quantum evolution operator, one finds the following formal coherent state phase space path integral representation of the quantum evolution operator,

$$\langle q_f, p_f|U(t_f,t_i)|q_i,p_i\rangle = \int_{(q_i,p_i)}^{(q_f,p_f)} \left[\frac{\mathcal{D}q\mathcal{D}p}{2\pi\hbar}\right] \, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\left[\frac{1}{2}(\dot{q}p - q\dot{p}) - H(q,p)\right]}, \tag{330}$$

corresponding to the following exact and explicit construction,

$$\begin{aligned} &\langle q_f, p_f|U(t_f,t_i)|q_i,p_i\rangle = \lim_{N\to\infty} \int_{-\infty}^{+\infty} \prod_{\alpha=1}^{N-1} \tfrac{dq_\alpha dp_\alpha}{2\pi\hbar} \times \\ &\times \exp\left\{\tfrac{i}{\hbar}\sum_{\alpha=0}^{N-1} \epsilon \left(\tfrac{1}{2}\left[\tfrac{q_{\alpha+1}-q_\alpha}{\epsilon} p_\alpha \, - \, q_\alpha \tfrac{p_{\alpha+1}-p_\alpha}{\epsilon}\right] \, - \, h_\alpha \, + \, \tfrac{1}{4} i\epsilon \left[\lambda \left(\tfrac{q_{\alpha+1}-q_\alpha}{\epsilon}\right)^2 \, + \, \tfrac{1}{\lambda}\left(\tfrac{p_{\alpha+1}-p_\alpha}{\epsilon}\right)^2\right]\right)\right\}, \end{aligned} \tag{331}$$

where

$$h_\alpha = \frac{\langle q_{\alpha+1}, p_{\alpha+1}|\hat{H}|q_\alpha,p_\alpha\rangle}{\langle q_{\alpha+1}, p_{\alpha+1}|q_\alpha,p_\alpha\rangle}. \tag{332}$$

Note that in contradistinction to the previous path integral representations, in the coherent state phase space one all phase space variables are treated identically; there are as many of the q as of the p type, all integrated over with the Liouville measure in phase space. Nevertheless, the path integral remains non invariant under phase space canonical transformations, nor is it invariant under changes of coordinates in configuration space.

4.6 The nonrelativistic charged particle in a background electromagnetic field

From a previous discussion of that system, we know that the classical Hamiltonian for a charged nonrelativistic particle subjected to an electromagnetic field, described by the scalar and vector gauge potentials $\Phi(t,\vec{r})$ and $\vec{A}(t,\vec{r})$, as well as to conservative forces of total potential energy $V(\vec{r})$, is given by

$$H = \frac{1}{2m}\left[\vec{p} - q\vec{A}(t,\vec{r})\right]^2 + q\Phi(t,\vec{r}) + V(\vec{r}), \tag{333}$$

the cartesian coordinates of the phase space variables $(\vec{r},\vec{p})$ being canonically conjugate with the canonical Poisson brackets $\left\{x^i, p_j\right\} = \delta^i_j$ $(i,j=1,2,3)$. Here m and q denote of course the mass and charge of the particle, respectively.

According to the correspondence principle of canonical quantisation, the quantum Hamiltonian of this system is then

$$\hat{H} = \frac{1}{2m}\left[\vec{\hat{p}} - q\vec{A}(t,\vec{\hat{r}})\right]^2 + q\Phi(t,\vec{\hat{r}}) + V(\vec{\hat{r}}), \tag{334}$$

in which now the quantum operators $\vec{\hat{r}}$ and $\vec{\hat{p}}$ have the following commutation relations for their cartesian coordinates, $[\hat{x}^i, \hat{p}_j] = i\hbar\delta^i_j$, it being understood that these are also (preferably) self-adjoint operators on the space of quantum states, thus defining a 3-fold tensor product (over the cartesian components) of the Heisenberg algebra over $\mathbb{R}$.

Since the physical space in which the particle is moving is assumed to be the Euclidean space $\mathbb{R}^3$, there exists essentially a unique representation of that algebra, given for instance in terms of the configuration space wave function representation of states, $\psi(t,\vec{r}) = \langle\vec{r}|\psi,t\rangle$, in which case the operators $\vec{\hat{r}}$ and $\vec{\hat{p}}$ have the following functional representations

$$\langle\vec{r}|\vec{\hat{r}}\,|\psi,t\rangle = \vec{r}\,\psi(t,\vec{r}), \qquad \langle\vec{r}|\vec{\hat{p}}\,|\psi,t\rangle = -i\hbar\vec{\nabla}\psi(t,\vec{r}). \tag{335}$$

By direct substitution into the above abstract quantum Hamiltonian, the Schrödinger equation in configuration space then reads,

$$\left\{-\frac{\hbar^2}{2m}\left[\vec{\nabla}-i\frac{q}{\hbar}\vec{A}(t,\vec{r})\right]^2 \,+\, q\Phi(t,\vec{r}) \,+\, V(\vec{r})\right\}\,\psi(t,\vec{r}) = i\hbar\frac{\partial\psi(t,\vec{r})}{\partial t}. \tag{336}$$

It is also possible to express the same quantum dynamics in the following form,

$$\left\{-\frac{\hbar^2}{2m}\left[\vec{\nabla}-i\frac{q}{\hbar}\vec{A}(t,\vec{r})\right]^2 \,+\, V(\vec{r})\right\}\,\psi(t,\vec{r}) = i\hbar\left[\frac{\partial}{\partial t}+i\frac{q}{\hbar}\Phi(t,\vec{r})\right]\,\psi(t,\vec{r}). \tag{337}$$

This form of the Schrödinger equation is most relevant to study the issue of its possible invariance under the gauge transformations of the electromagnetic potentials,

$$\Phi'(t,\vec{r}) = \Phi(t,\vec{r}) - \partial_t\chi(t,\vec{r}), \qquad \vec{A}'(t,\vec{r}) = \vec{A}(t,\vec{r}) + \vec{\nabla}\chi(t,\vec{r}), \tag{338}$$

$\chi(t,\vec{r})$ being an arbitrary function of time and space. It is clear that since these potentials contribute to the Schrödinger equation in combination with time or space derivatives, if there is any chance to identify these transformations also as a symmetry of the Schrödinger equation, the quantum wave function has to transform accordingly with a phase factor. After but only a little reflection, one quickly comes to the conclusion that the appropriate transformation of the quantum wave function in configuration space is

$$\psi'(t,\vec{r}) = e^{i\frac{q}{\hbar}\chi(t,\vec{r})}\,\psi(t,\vec{r}). \tag{339}$$

Indeed, one then finds that each of the terms involving the time or space derivatives and the scalar and vector gauge potentials transforms as follows,

$$\begin{aligned}
\left[\vec{\nabla}-i\frac{q}{\hbar}\vec{A}'(t,\vec{r})\right]\,\psi'(t,\vec{r}) &= e^{i\frac{q}{\hbar}\chi(t,\vec{r})}\,\left[\vec{\nabla}-i\frac{q}{\hbar}\vec{A}(t,\vec{r})\right]\,\psi(t,\vec{r}),\\
\left[\partial_t+i\frac{q}{\hbar}\Phi'(t,\vec{r})\right]\,\psi'(t,\vec{r}) &= e^{i\frac{q}{\hbar}\chi(t,\vec{r})}\,\left[\partial_t+i\frac{q}{\hbar}\Phi(t,\vec{r})\right]\,\psi(t,\vec{r}).
\end{aligned} \tag{340}$$

Consequently, both sides of the Schrödinger equation vary with the same phase factor as the wave function, thus leaving the equation *in fine* invariant indeed under the local gauge symmetry of the electromagnetic interaction.

Note that the actual transformation associated to the symmetry is that through the phase factor. Indeed, introducing

$$U(t,\vec{r}) = e^{i\frac{q}{\hbar}\chi(t,\vec{r})}, \tag{341}$$

one may write

$$\begin{aligned}
\psi'(t,\vec{r}) &= U(t,\vec{r})\,\psi(t,\vec{r}),\\
\Phi'(t,\vec{r}) &= U(t,\vec{r})\,\Phi(t,\vec{r})\,U^{-1}(t,\vec{r}) \,-\, i\frac{\hbar}{q}\,U(t,\vec{r})\,\partial_t\,U^{-1}(t,\vec{r}),\\
\vec{A}'(t,\vec{r}) &= U(t,\vec{r})\,\vec{A}(t,\vec{r})\,U^{-1}(t,\vec{r}) \,+\, i\frac{\hbar}{q}\,U(t,\vec{r})\,\vec{\nabla}\,U^{-1}(t,\vec{r}),
\end{aligned} \tag{342}$$

a form which readily extends to nonabelian symmetries for which $U(t,\vec{r})$ then stands for elements of some nonabelian symmetry group. In the present case the symmetry group is thus that of phase transformations, or rotations of the unit circle in the complex plane, or simply the group U(1) of 1×1 unitary matrices such that $U^\dagger = U^{-1}$, namely complex numbers of unit norm, thus pure phases. Hence the electromagnetic interaction is intimately connected the local gauge symmetry based on the group U(1).

In fact in the above expressions (340) lies hidden one of the two secrets necessary to construct in general Yang-Mills theories of the abelian and nonabelian type. Note that for a constant phase transformation, $\chi(t,\vec{r}) = \chi_0$, the wave function $\psi(t,\vec{r})$ and its time and space derivatives transform in a similar fashion, simply being multiplied by the same phase factor. However when the symmetry is made local, namely when $\chi(t,\vec{r})$ becomes an arbitrary function of time and space, the ordinary time and space derivatives of the wave function do no longer transform in the same covariant way under the phase symmetry as

does the wave function itself. There is always one more contribution,

$$\begin{aligned}\partial_t\, e^{i\frac{q}{\hbar}\chi(t,\vec{r})}\,\psi(t,\vec{r}) &= e^{i\frac{q}{\hbar}\chi(t,\vec{r})}\left[\partial_t\,\psi(t,\vec{r}) + i\frac{q}{\hbar}\partial_t\chi(t,\vec{r})\psi(t,\vec{r})\right],\\ \vec{\nabla}\, e^{i\frac{q}{\hbar}\chi(t,\vec{r})}\,\psi(t,\vec{r}) &= e^{i\frac{q}{\hbar}\chi(t,\vec{r})}\left[\vec{\nabla}\psi(t,\vec{r}) + i\frac{q}{\hbar}\vec{\nabla}\chi(t,\vec{r})\psi(t,\vec{r})\right].\end{aligned} \tag{343}$$

These additional terms are precisely those that are cancelled by the transformation of the gauge potentials in the combinations

$$\left[\partial_t - i\frac{q}{\hbar}\Phi(t,\vec{r})\right]\psi(t,\vec{r}), \qquad \left[\vec{\nabla} + i\frac{q}{\hbar}\vec{A}(t,\vec{r})\right]\psi(t,\vec{r}). \tag{344}$$

These types of extended or generalised derivatives are known as **covariant derivatives**, since when acting on an object transforming covariantly under a symmetry they produce again a quantity covariant for the same transformations, in contradistinction to the ordinary derivatives.

Incidentally, there is a difference in sign in the contributions of the electromagnetic gauge potentials to the time and space covariant derivatives. This difference in sign is directly related to the opposite sign in the time and space contributions to the spacetime metric, $(ct)^2 - \vec{r}^{\,2}$, of Minkowski spacetime in special relativity. Indeed, the electromagnetic interaction is also explicitly invariant under the symmetry group of that geometry, namely the Lorentz and Poincaré groups. Thus the germs of two of the most important insights of XX$^{\text{th}}$ century physics, namely special relativity and the fundamental rôle of the gauge symmetry principle as governing all fundamental interactions, are already present in the Schrödinger equation of the nonrelativistic charged particle in a background electromagnetic field.

4.7 The two dimensional spherically symmetric harmonic oscillator

The Lagrange function of the spherically symmetric harmonic oscillator of angular frequency ω and mass m, in two dimensional Euclidean space, is

$$L = \frac{1}{2}m\left(\dot{x}_1^2 + \dot{x}_2^2\right) - \frac{1}{2}m\omega^2\left(x_1^2 + x_2^2\right), \tag{345}$$

x_1 and x_2 being the cartesian coordinates representing the two degrees of freedom of this dynamics. As such, this system is literally the sum of two independent one dimensional harmonic oscillators. One may thus simply take over all the results from previous discussions of the classical and quantum harmonic oscillator, and add an index $\alpha = 1, 2$ to the variables, and finally sum over these, which at the quantum level means taking the ordinary tensor product of the two spaces of quantum states.

Consequently, we know that the Hamiltonian of the system is simply,

$$H = \frac{1}{2m}\left(p_1^2 + p_2^2\right) + \frac{1}{2}m\omega^2\left(x_1^2 + x_2^2\right), \tag{346}$$

p_1 and p_2 being of course the momenta canonically conjugate to the coordinates x_1 and x_2, respectively. At the quantum level, one has the two pairs of operators $\hat{x}_1$ and $\hat{p}_1$, on the one hand, and $\hat{x}_2$ and $\hat{p}_2$ on the other hand, with each pair obeying the Heisenberg algebra, $[\hat{x}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}$ $(\alpha, \beta = 1, 2)$. Introducing the associated creation and annihilation operators, we thus have,

$$\begin{aligned} a_1 &= \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x}_1 + \frac{i}{m\omega}\hat{p}_1\right], \qquad a_1^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x}_1 - \frac{i}{m\omega}\hat{p}_1\right],\\ a_2 &= \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x}_2 + \frac{i}{m\omega}\hat{p}_2\right], \qquad a_2^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left[\hat{x}_2 - \frac{i}{m\omega}\hat{p}_2\right],\end{aligned} \tag{347}$$

obeying the tensor product Fock algebra,

$$[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}\mathbb{I}. \tag{348}$$

Conversely,

$$\begin{aligned} \hat{x}_1 &= \sqrt{\frac{\hbar}{2m\omega}}\left[a_1 + a_1^\dagger\right], \qquad \hat{p}_1 = -im\omega\sqrt{\frac{\hbar}{2m\omega}}\left[a_1 - a_1^\dagger\right],\\ \hat{x}_2 &= \sqrt{\frac{\hbar}{2m\omega}}\left[a_2 + a_2^\dagger\right], \qquad \hat{p}_2 = -im\omega\sqrt{\frac{\hbar}{2m\omega}}\left[a_2 - a_2^\dagger\right].\end{aligned} \tag{349}$$

Obviously, the quantum Hamiltonian then reads

$$\hat{H} = \hbar\omega \left(a_1^\dagger a_1 + \frac{1}{2} \right) + \hbar\omega \left(a_2^\dagger a_2 + \frac{1}{2} \right) = \hbar\omega \left(a_1^\dagger a_1 + a_2^\dagger a_2 + 1 \right). \tag{350}$$

Introducing the orthonormalised Fock state basis

$$|n_1, n_2\rangle = \frac{1}{\sqrt{n_1!\, n_2!}} \left(a_1^\dagger \right)^{n_1} \left(a_2^\dagger \right)^{n_2} |0,0\rangle, \qquad \langle n_1, n_2 | n_1', n_2' \rangle = \delta_{n_1 n_1'} \delta_{n_2 n_2'}, \tag{351}$$

it is clear that these states also diagonalise the Hamiltonian with the following energy spectrum,

$$\hat{H}|n_1, n_2\rangle = E(n_1, n_2)\, |n_1, n_2\rangle, \qquad E(n_1, n_2) = \hbar\omega \left(n_1 + n_2 + 1 \right). \tag{352}$$

However, this spectrum is degenerate at each level except for the ground state at $(n_1, n_2) = (0, 0)$. Indeed, at a given energy level $E(n_1, n_2) = \hbar\omega(N + 1)$ with $N = 0, 1, 2 \ldots$, we have as many states as there are partitions of the natural number N in two natural numbers n_1 and n_2, namely $(N+1)$ states. There must exist an actual solid and sound explanation for this fact. It cannot be just a mere numerical coincidence. The first thought that comes to one's mind is that of a symmetry.

Certainly, the system is invariant under rotations in the plane, and indeed it possesses a conserved angular-momentum (perpendicular to the plane),

$$L_3 = x_1 p_2 - x_2 p_1. \tag{353}$$

At the quantum level and expressed in terms of the creation and annihilation operators, one has the operator,

$$\hat{L}_3 = -i\hbar \left(a_1^\dagger a_2 - a_2^\dagger a_1 \right). \tag{354}$$

From this expression, even though the operators $\hat{H}$ and $\hat{L}_3$ commute, the Fock space basis $|n_1, n_2\rangle$ does not diagonalise them both. We need to find another basis of Hilbert space which diagonalises these two commuting operators.

For this purpose, let us introduce an helicity basis as follows,

$$\begin{aligned}
a_\pm &= \frac{1}{\sqrt{2}} \left[a_1 \mp i a_2 \right], \qquad a_\pm^\dagger = \frac{1}{\sqrt{2}} \left[a_1^\dagger \pm i a_2^\dagger \right], \\
a_1 &= \frac{1}{\sqrt{2}} \left[a_+ + a_- \right], \qquad a_1^\dagger = \frac{1}{\sqrt{2}} \left[a_+^\dagger + a_-^\dagger \right], \\
a_2 &= \frac{i}{\sqrt{2}} \left[a_+ - a_- \right], \qquad a_2^\dagger = -\frac{i}{\sqrt{2}} \left[a_+^\dagger - a_-^\dagger \right],
\end{aligned} \tag{355}$$

such that

$$[a_\pm, a_\pm^\dagger] = \mathbb{I}, \qquad [a_\pm, a_\mp^\dagger] = 0. \tag{356}$$

These redefinitions in turn imply

$$\begin{aligned}
\hat{x}_1 &= \frac{1}{2} \sqrt{\frac{\hbar}{m\omega}} \left[a_+ + a_- + a_+^\dagger + a_-^\dagger \right], \qquad \hat{p}_1 = -i \frac{m\omega}{2} \sqrt{\frac{\hbar}{m\omega}} \left[a_+ + a_- - a_+^\dagger - a_-^\dagger \right], \\
\hat{x}_2 &= \frac{i}{\sqrt{2}} \sqrt{\frac{\hbar}{m\omega}} \left[a_+ - a_- - a_+^\dagger + a_-^\dagger \right], \qquad \hat{p}_2 = \frac{m\omega}{2} \sqrt{\frac{\hbar}{m\omega}} \left[a_+ - a_- + a_+^\dagger - a_-^\dagger \right],
\end{aligned} \tag{357}$$

hence

$$\hat{x}_\pm = \hat{x}_1 \pm i\hat{x}_2 = \sqrt{\frac{\hbar}{m\omega}} \left[a_\mp + a_\pm^\dagger \right], \qquad \hat{p}_\pm = \frac{1}{2} \left[\hat{p}_1 \mp i\hat{p}_2 \right] = -\frac{im\omega}{2} \sqrt{\frac{\hbar}{m\omega}} \left[a_\pm - a_\mp^\dagger \right], \tag{358}$$

which are such that

$$[\hat{x}_\pm, \hat{p}_\pm] = i\hbar, \qquad [\hat{x}_\pm, \hat{p}_\mp] = 0. \tag{359}$$

One then also finds

$$\begin{aligned}\hat{H} &= \hbar\omega\left(a_+^\dagger a_+ + a_-^\dagger a_- + 1\right),\\ \hat{L}_3 &= \hbar\left(a_+^\dagger a_+ - a_-^\dagger a_-\right).\end{aligned} \tag{360}$$

Hence by considering rather the orthonormalised Fock space helicity basis

$$|n_+, n_-\rangle = \frac{1}{\sqrt{n_+!\, n_-!}}\left(a_+^\dagger\right)^{n_+}\left(a_-^\dagger\right)^{n_-}|0,0\rangle, \qquad \langle n_+, n_-|n'_+, n'_-\rangle = \delta_{n_+ n'_+}\,\delta_{n_- n'_-}, \tag{361}$$

based on the alternative Fock algebra $(a_\pm, a_\pm^\dagger)$, one has indeed diagonalised both operators,

$$\begin{aligned}\hat{H}|n_+, n_-\rangle &= E(n_+, n_-)|n_+, n_-\rangle, \qquad E(n_+, n_-) = \hbar\omega(n_+ + n_- + 1),\\ \hat{L}_3|n_+, n_-\rangle &= \hbar(n_+ - n_-)|n_+, n_-\rangle.\end{aligned} \tag{362}$$

The previously described degeneracy of energy levels is again observed in terms of $N = n_+ + n_-$. However the angular-momentum operator does not map states belonging to a same level into one another. Hence, the degeneracy cannot be related to that symmetry under SO(2)=U(1) rotations in the plane. A larger symmetry must be at play. Note that the quanta of the $a_+^\dagger$ type carry a unit $(+\hbar)$ of angular-momentum, whereas those of type $a_-^\dagger$ carry a unit $(-\hbar)$ of angular-momentum. The combinations of the degrees of freedom which defined these quantities are indeed associated to the helicities $(+1)$ and (-1) of the oscillating modes of the system.

Both operators $\hat{H}$ and $\hat{L}_3$ may be written in the form,

$$\hat{H} = \hbar\omega\begin{pmatrix} a_+^\dagger & a_-^\dagger\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix} a_+\\ a_-\end{pmatrix} + \hbar\omega, \qquad \hat{L}_3 = \hbar\begin{pmatrix} a_+^\dagger & a_-^\dagger\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix} a_+\\ a_-\end{pmatrix}. \tag{363}$$

From that point of view, it should be quite clear that any SU(2) unitary transformation, namely a 2×2 matrix U over $\mathbb{C}$ which is unitary, $U^\dagger = U^{-1}$, and of unit determinant, $\det U = 1$, and acting on the pair of annihilation operators as

$$\begin{pmatrix} a_+\\ a_-\end{pmatrix} \longrightarrow \begin{pmatrix} a'_+\\ a'_-\end{pmatrix} = U\begin{pmatrix} a_+\\ a_-\end{pmatrix}, \tag{364}$$

leaves the Hamiltonian invariant. In other words, there is a larger symmetry present in the system than simply the SO(2)=U(1) symmetry of rotations which on the pair of annihilation operators act as

$$U = \begin{pmatrix} e^{i\alpha} & 0\\ 0 & e^{-i\alpha}\end{pmatrix}, \tag{365}$$

α being a rotation angle. Note that the latter remark also shows that the symmetry SU(2) includes as a subgroup the SO(2)=U(1) symmetry under rotations in the plane. This larger SU(2) symmetry is an example of what is called a **dynamical symmetry**, namely a symmetry of the Hamiltonian formulation of the system which is not one of its Lagrangian formulation. Such a situation is indeed possible *a priori* since the Hamiltonian formulation involves both the configuration space coordinates and their conjugate momenta which may therefore mix under a symmetry transformation, a situation which is not possible in the Lagrangian formulation involving the configuration space coordinates only.

Let us see whether we may introduce now, based on the Fock algebra generators $a_\pm^\dagger$ and $a_\pm$, operators which map states into one another within a same energy level, thus still commuting with the Hamiltonian, and then determine their algebra. The obvious candidates are,

$$T_+ = a_+^\dagger a_-, \qquad T_- = a_-^\dagger a_+, \qquad T_3 = \frac{1}{2}\left(a_+^\dagger a_+ - a_-^\dagger a_-\right) = \frac{1}{2\hbar}\hat{L}_3. \tag{366}$$

It takes but only a little calculation to obtain

$$[T_+, T_-] = 2T_3, \qquad [T_3, T_\pm] = \pm T_\pm, \qquad [\hat{H}, T_\pm] = 0, \qquad [\hat{H}, T_3] = 0. \tag{367}$$

Introducing now

$$T_1 = \frac{1}{2}\,(T_+ + T_-)\,, \qquad T_2 = -\frac{i}{2}\,(T_+ - T_-)\,, \qquad T_\pm = T_1 \pm iT_2, \tag{368}$$

the same algebra reads

$$[T_i, T_j] = i\epsilon_{ijk}\,T_k, \qquad i,j,k = 1,2,3, \tag{369}$$

ϵ_{ijk} being the totally antisymmetric invariant tensor in three dimensions with $\epsilon_{123} = +1$. The last set of commutation relations is directly identified with the SU(2) algebra, or also the SO(3) algebra which as algebras are identical (but not as groups since SO(3)=SU(2)/$\mathbb{Z}_2$ as a quotient of groups). One famous finite dimensional representation of that algebra is given by the 2×2 Pauli matrices $T_i = \frac{1}{2}\sigma_i$, with

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{370}$$

Let us now turn to the action of the operators $T_\pm$ on the Fock basis states $|n_+, n_-\rangle$. Since for a single harmonic oscillator one has

$$a|n\rangle = \sqrt{n}|n-1\rangle, \qquad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{371}$$

it follows that

$$\begin{aligned} T_+|n_+, n_-\rangle &= \sqrt{(n_+ + 1)n_-}\;|n_+ + 1, n_- - 1\rangle, \\ T_-|n_+, n_-\rangle &= \sqrt{n_+(n_- + 1)}\;|n_+ - 1, n_- + 1\rangle, \\ T_3|n_+, n_-\rangle &= \frac{1}{2}(n_+ - n_-)\,|n_+, n_-\rangle, \end{aligned} \tag{372}$$

showing that indeed it is this algebra of operators which accounts for the degeneracy of the energy levels. Let us introduce the following representation for the helicity occupation numbers $n_\pm$,

$$n_+ + n_- = N = 2j, \qquad n_+ - n_- = 2m, \qquad \frac{1}{2}\,(n_+ - n_-) = m, \tag{373}$$

hence

$$n_+ = j + m, \qquad n_- = j - m, \tag{374}$$

where j thus takes positive integer or half-integer values according to whether the energy level N is even or odd, while m takes values between j and $(-j)$ in unit steps, $-j \leq m \leq j$ (m thus measures the T_3 eigenvalue, or half the angular-momentum eigenvalue L_3 in units of $\hbar$). The above actions then read

$$T_+|j,m\rangle = \sqrt{(j-m)(j+m+1)}\,|j,m+1\rangle, \qquad T_-|j,m\rangle = \sqrt{(j+m)(j-m+1)}\,|j,m-1\rangle, \tag{375}$$

with $|j,m\rangle = |n_+, n_-\rangle$ given the above correspondence between these integer or half-integer variables.

In conclusion, for a given energy level $N = 0, 1, 2, \ldots$, one obtains a certain SU(2) representation as a finite $N + 1 = 2j + 1$ dimensional subspace of the complete Hilbert space of quantum states of this system. This representation is characterised by the single integer or half-integer number j, known as the **spin** of that representation, whereas the states within that representation of given spin j are distinguished by their T_3 eigenvalue m lying between $(-j)$ and j in integer steps, with the above matrix elements for the action of the two other operators $T_\pm$ of the SU(2) algebra. As a matter of fact, we have in this manner recovered **all** finite dimensional representations of the symmetry algebra SU(2), which is also the algebra of the symmetry group SO(3) of rotations in three dimensional Euclidean space. The above formula for the action of $T_\pm$ and T_3 in a given spin j representation are valid as such in full generality, independently of the system in which these symmetries may be realised. Any rotationally invariant system in three dimensions will find its quantum states organised according to these spin representations of SU(2). But it is matter of experiment to determine which spin values are realised for a specific physical system. For example, that the electron has spin 1/2 may only be determined experimentally.

As an illustration, consider the value $N = 1$ or $j = 1/2$, namely the first excited state of the present system. It is thus doubly degenerated, with

$$T_3\left|j = \frac{1}{2}, m = \frac{1}{2}\right\rangle = \frac{1}{2}\left|j = \frac{1}{2}, m = \frac{1}{2}\right\rangle, \qquad T_3\left|j = \frac{1}{2}, m = -\frac{1}{2}\right\rangle = -\frac{1}{2}\left|j = \frac{1}{2}, m = -\frac{1}{2}\right\rangle, \tag{376}$$

$$T_+ \left| j = \frac{1}{2}, m = \frac{1}{2} \right\rangle = 0, \qquad T_+ \left| j = \frac{1}{2}, m = -\frac{1}{2} \right\rangle = \left| j = \frac{1}{2}, m = \frac{1}{2} \right\rangle, \tag{377}$$

$$T_- \left| j = \frac{1}{2}, m = \frac{1}{2} \right\rangle = \left| j = \frac{1}{2}, m = -\frac{1}{2} \right\rangle, \qquad T_- \left| j = \frac{1}{2}, m = -\frac{1}{2} \right\rangle = 0, \tag{378}$$

and the associations $\left|j = \frac{1}{2}, m = \frac{1}{2}\right\rangle = |n_+ = 1, n_- = 0\rangle$, $\left|j = \frac{1}{2}, m = -\frac{1}{2}\right\rangle = |n_+ = 0, n_- = 1\rangle$. In other words, in this two dimensional basis, the matrix representation of the operators T_3 and $T_\pm$ is given precisely by the Pauli matrices. Clearly, the ground state of the system, $|j = 0, m = 0\rangle = |n_+ = 0, n_- = 0\rangle$, corresponds to a trivial representation of the SU(2) algebra for which $T_3 = 0$ and $T_\pm = 0$.

5 Symmetries and the First Noether Theorem

5.1 Motivation

Symmetries play a central rôle nowadays in fundamental and more applied physics, not only as means for solving otherwise analytically intractable problems but more importantly, as providing profound insight into properties of interactions and of conservation laws. Indeed, when it comes to a continuous symmetry associated to the notion of a Lie group, Noether's first theorem establishes a direct relation between the existence of such continuous symmetries and that of conserved quantities, often also called **Noether charges**. Furthermore within the Hamiltonian formulation the algebra of Poisson brackets of these Noether charges proves to be identical to the abstract algebra of the Lie symmetry group of which the charges are then the generators. In other words the abstract algebra of the Lie symmetry group is then realised on the phase space of the system through the conserved quantities and their Poisson brackets. When canonical quantisation may proceed in a manner consistent with the Lie algebra of symmetries, the associated quantum operators then generate, as linear transformations, the symmetry algebra on the quantum space of states. Consequently, the latter Hilbert space then provides a linear representation of the Lie algebra. It is here that the whole of Lie algebra representation theory becomes most relevant, with in particular a classification of the possible quantum representations of a given classical symmetry. As an example, if a system is invariant under SO(3) rotations in three Euclidean space dimensions, the Noether charges correspond to the total angular-momentum vector of that system, of which the Poisson brackets are isomorphic to the Lie algebra $so(3)$ of that Lie group. When quantised, one then is able to classify the quantum space of states in terms of representations of $so(3)$, namely also $su(2)$, since the algebras of SO(3) and SU(2) are identical. The representations of SU(2) are labelled in terms of the spin value j taking an integer or half-integer positive value (these representations were introduced in the context of the two dimensional spherically symmetric harmonic oscillator in the previous Section). This fundamental result based on Noether's first theorem is especially important when the symmetry group is a compact Lie group, since all finite dimensional and unitary representations of all compact Lie groups have been classified, one of the towering achievements of pure algebra in XX$^{\text{th}}$ century mathematics. But this is not the purpose of the present notes.

The situation just described is also the generic one, when it comes to continuous Lie symmetries, namely a group of transformations defined in terms of a collection of continuous parameters. A system may also be invariant under a discrete symmetry of which the group elements depend on a collection of parameters taking only a discrete set of values. As an example, consider a square in the plane. Its symmetry group is a specific subgroup of O(2) or SO(2), namely those rotations by $\pm\pi/2$ radians modulo a reflection in the origin of one of the coordinate axes. There are no conserved quantities, or Noether charges associated to a discrete symmetry, even though such a symmetry does impose some restrictions or relations between physical quantities, of relevance especially when it comes to the quantum world. Famous symmetries of that type are those of space parity, P, time reversal, T, and charge conjugation, C, the latter corresponding to the exchange of particles with their antiparticles.

In these notes we shall not discuss discrete symmetries, but focus only on Noether's first theorem. There exist still one or two more Noether theorems, in relation with gauge symmetries. As was illustrated through the example of the electromagnetic interaction in previous Sections, a gauge symmetry is a continuous Lie symmetry of which the continuous parameters themselves may be continuous functions of time or even spacetime (the latter in a field theory context). As such, when as a particular case one takes for these

function parameters just constant values, one has what is also often called a **global symmetry**. This is the situation addressed above, corresponding to Noether's first theorem, leading to conserved Noether charges. However, in the eventuality of a local or gauged symmetry, Noether's second and third theorems imply even further restrictions on the Noether charges and other quantities that are involved in the gauge symmetry transformations, which are of relevance to the quantisation of gauge invariant systems. In particular, Noether's second theorem implies that for configurations of the system which are "physical" in the sense of being indeed gauge invariant, the Noether charges of the gauge symmetries have to vanish altogether. Given the previous remark that Noether charges are the generators of the symmetries of which they are the conserved quantities, indeed they would need to vanish in the case of gauge invariant configurations. In these notes we shall not discuss Noether's second and third theorem (for those interested, a discussion may be found in Ref. [3]).

This much having been said, it is necessary to specify what is exactly meant by a symmetry. Clearly it must consist in a transformation of the configuration space variables, q^n, of the system, and possibly even in combination with a transformation in the time variable[17], t, of the form

$$t' = t'(t), \qquad q^{n\prime}(t') = q^{n\prime}\left(q^n, t\right). \tag{379}$$

In the case of a discrete symmetry the functions $t'(t)$ and $q^{n\prime}\left(q^n, t\right)$ would depend on a collection of parameters taking values in a discrete set (*viz.*, the example of the symmetries of the square). In the case of a continuous symmetry forming a Lie group, the symmetry parameters take their values in a continuous set. For instance, the two or three dimensional spherically symmetric harmonic oscillator is invariant under all space rotations. These form the Lie groups SO(2) or SO(3), respectively, and their elements may be characterised in terms of angular variables, the rotation angle in the plane in the first case, or the three Euler angles in the second case, each of these angular variables taking values in continuous albeit finite intervals. So far these precisions only concern the transformation, but when does it qualify as a symmetry?

Contrary may be to everyday's usage of the word which is taken to mean that something is symmetric under a transformation if it is left invariant under that transformation (such as the square of the above example), in the context of physics and the dynamics of systems, what one means by the concept of symmetry is not that a particular configuration of the system is left invariant by the transformation (say, only when a set of particles occupies a preselected collection of points in space does there exist a particular symmetry), but rather **that the space of solutions to its equations of motion is left invariant under the symmetry transformation**. In other words, a symmetry is a transformation which maps any given solution to the equations of motion into another solution to the same equations of motion. Often, one says that a symmetry leaves the equations of motion form invariant. This means that when expressing the equations of motion in terms of the not-yet-transformed variables or the transformed ones, the functional relations between these variables in each case are identical, *i.e.*, that they have the same form. Given the above representation of such a transformation, this means that when expressed in terms of the variables carrying a prime, t' and $q^{n\prime}$, the equations they obey are the same as those for the variables not carrying that prime, namely t and q^n. One may easily imagine examples for oneself's, and a few will be discussed hereafter.

Since our discussion is rooted in the variational principle, how then does the action of a system transform under a symmetry? Since the equations of motion are form invariant, necessarily under a symmetry the action may only change by a total time derivative. Indeed as is well known actions that differ only by a total time derivative share identical equations of motion. Hence when transformations of the above class define a symmetry of a dynamics, the action of the system must transform according to

$$S[q^{n\prime}] = \int dt'\, L\left(q^{n\prime}, \frac{dq^{n\prime}}{dt'}\right) = \int dt \left[L\left(q^n, \frac{dq^n}{dt}\right) + \frac{d\Lambda(q^n, t)}{dt}\right], \tag{380}$$

where $\Lambda(q^n, t)$ is some function implicitly defined through the transformation of the action under the symmetry. In particular, it depends on the parameters of the symmetry group, say the rotation angles in the case of a rotational symmetry in space. Using then the composition law for differentials,

$$dt' = dt\, \frac{dt'}{dt}, \tag{381}$$

[17] Why not for instance redefine time by an arbitrary shift of t_0?

a system is invariant under a symmetry transformation if its Lagrange function changes according to

$$\frac{dt'}{dt}\,L\left(q^{n\prime},\frac{dt}{dt'}\,\frac{dq^{n\prime}}{dt}\right)=L\left(q^n,\frac{dq^n}{dt}\right)\,+\,\frac{d\Lambda\left(q^n,t\right)}{dt}. \tag{382}$$

Note that in the case of a field theory where the action is given as the spacetime integral of the Lagrangian density $\mathcal{L}$, the above total time derivative may be replaced by a total surface term, namely a total spacetime divergence. In the presence of nontrivial topology in space such contributions may be physically relevant for some symmetries, leading at the quantum level to quantisation rules on some parameters. A noteworthy example of this are supersymmetric field theories; under a supersymmetry transformation, which exchanges bosons and fermions (states of integer and half-integer spin), the Lagrangian density varies precisely always by a total surface term.

The discussion so far, including the property (382), applies whether the symmetry is a continuous or a discrete one. Let us now restrict to a set of transformations forming a Lie group, namely a continuous symmetry.

5.2 Linearisation of a Lie symmetry group

In the case of a continuous group of symmetry transformations, at least for the component of the group connected to the identity transformation, one may consider infinitesimal transformations, namely transformations in a linearised form, simply by linearising the transformations in the parameters of the group. Hence let us now consider transformations of the following form,

$$t'=t+\delta t(t),\qquad q^{n\prime}=q^n+\delta q^n\left(q^n,t\right),\qquad \Lambda=\delta\Lambda\left(q^n,t\right), \tag{383}$$

with $\delta t(t)$ and $\delta q^n(q^n,t)$ some infinitesimal (or linearised) variations of the variables t and q^n possessing the indicated dependencies on t and q^n. Since in the absence of a transformation no total time derivative term is induced in the action, the function $\Lambda(q^n,t)$ has no zeroth order contribution, while the function $\delta\Lambda(q^n,t)$ is determined from the knowledge of $\Lambda(q^n,t)$ and its dependence on the group parameters, given a symmetry.

All that is required now is to substitute these variations in the variables in the fundamental identity (382), and expand the latter to first order in the quantities δt, δq^n and $\delta\Lambda$. It takes only a little calculation detailed hereafter to establish that for linearised continuous symmetries one has the following fundamental Noether identity,

$$\left[\delta q^n-\delta t\,\dot{q}^n\right]\left[\frac{\partial L}{\partial q^n}\,-\,\frac{d}{dt}\,\frac{\partial L}{\partial\dot{q}^n}\right]\,+\,\frac{d}{dt}\left[\delta t\left(L-\dot{q}^n\frac{\partial L}{\partial\dot{q}^n}\right)\,+\,\delta q^n\frac{\partial L}{\partial\dot{q}^n}\,-\,\delta\Lambda\right]=0, \tag{384}$$

where once again the implicit summation rule over repeated indices is to be understood.

In order to establish this result, let us first note that we have, to first order in the variation $\delta t(t)$,

$$t'=t+\delta t(t),\qquad t=t'-\delta t(t),\qquad \frac{dt'}{dt}=1+\frac{d\delta t(t)}{dt},\qquad \frac{dt}{dt'}=1-\frac{d\delta t(t)}{dt}. \tag{385}$$

Consequently, again to first order the identity (382) reads

$$\left[1+\frac{d\delta t(t)}{dt}\right]\,L\left(q^n+\delta q^n,\left(1-\frac{d\delta t(t)}{dt}\right)\left(\frac{dq^n}{dt}+\frac{d\delta q^n}{dt}\right)\right)\,-\,L\left(q^n,\frac{dq^n}{dt}\right)=\frac{d\delta\Lambda}{dt}. \tag{386}$$

Expanded to first order we thus have

$$\frac{d\delta t(t)}{dt}L(q^n,\dot{q}^n)+\delta q^n\frac{\partial L}{\partial q^n}+\left[\frac{d\delta q^n}{dt}-\frac{d\delta t}{dt}\dot{q}^n\right]\frac{\partial L}{\partial\dot{q}^n}-\frac{d\delta\Lambda}{dt}=0. \tag{387}$$

Let us now bring as many terms as possible in the form of a total time derivative,

$$\begin{aligned}&\frac{d}{dt}\left[\delta tL+\delta q^n\frac{\partial L}{\partial\dot{q}^n}-\delta t\,\dot{q}^n\frac{\partial L}{\partial\dot{q}^n}-\delta\Lambda\right]\\&-\delta t\frac{dL}{dt}+\delta q^n\frac{\partial L}{\partial q^n}-\delta q^n\frac{d}{dt}\frac{\partial L}{\partial\dot{q}^n}+\delta t\,\frac{d}{dt}\left[\dot{q}^n\frac{\partial L}{\partial\dot{q}^n}\right]=0.\end{aligned} \tag{388}$$

Making explicit the contributions of the last line one finds

$$-\,\delta t\,\dot{q}^n\frac{\partial L}{\partial q^n}-\delta t\,\ddot{q}^n\frac{\partial L}{\partial \dot{q}^n}+\delta q^n\frac{\partial L}{\partial q^n}-\delta q^n\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^n}+\delta t\,\ddot{q}^n\frac{\partial L}{\partial \dot{q}^n}+\delta t\,\dot{q}^n\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^n}, \tag{389}$$

in which some terms cancel explicitly. As a consequence, the fundamental identity (384) is established.

What is truly remarkable about this result is that the Euler–Lagrange equations of motion appear explicitly in it, whereas all remaining terms contribute only through a total time derivative. Thus in particular, this implies that given any solution to the equations of motion there exists a quantity constructed out of the degrees of freedom of the system and their generalised velocities of which the total time derivative vanishes identically. In other words, as a consequence of the property (382) expressing the existence of a symmetry, in the case of a continuous symmetry there exist quantities which are conserved or constants of motion for any solution to the equations of motion of the system. In itself this is quite a remarkable result. However the identity (384) states something even stronger, namely that there exist specific combinations of the Euler–Lagrange equations of motion which reduce to total time derivatives. Let us make these remarks more specific by introducing now the collection of parameters of such Lie group symmetries.

5.3 The first Noether theorem: global Lie symmetry group

Let us now make explicit the parameters[18] α_a of the Lie group of which the transformations acting on the configurations q^n of the system and the time variable t define a symmetry of its dynamics in the sense of (382),

$$\delta t(t)=\alpha_a\,\chi^a(t),\qquad \delta q^n\,(q^n,t)=\alpha_a\,\phi^{an}\,(q^n,t)\,,\qquad \delta\Lambda\,(q^n,t)=\alpha_a\,\Lambda^a\,(q^n,t)\,. \tag{390}$$

Here $\chi^a(t)$, $\phi^{an}(q^n,t)$ and $\Lambda^a(q^n,t)$ are specific functions of the indicated variables, obtained from the functions $t'(t)$, $q^{n\prime}(q^n,t)$ and $\Lambda(q^n,t)$ by expanding these to first order in the group parameters α_a.

A direct substitution of these expansions in terms of the group parameters α_a into the fundamental Noether identity (384) clearly leads to **the First Noether identity**,

$$\frac{d\gamma^a}{dt}=[\phi^{an}\,-\,\chi^a\,\dot{q}^n]\,\left[\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^n}\,-\,\frac{\partial L}{\partial q^n}\right], \tag{391}$$

in which the **Noether charges** are given by

$$\gamma^a=\phi^{an}\,\frac{\partial L}{\partial \dot{q}^n}\,-\,\chi^a\left(\dot{q}^n\frac{\partial L}{\partial \dot{q}^n}\,-\,L\right)\,-\,\Lambda^a. \tag{392}$$

These identities, one for each independent value of the index a, namely each independent Lie group parameter hence generator, thus provide the statement of the first Noether theorem. If the Lie group G is of dimension N_G, there exist N_G independent linear combinations of the Euler–Lagrange equations of motion which are total time derivatives. As a corollary, it also follows that given any solution to the equations of motion there exist N_G quantities which are conserved, namely constants of motion of the system.

This conclusion is remarkable indeed. Lie symmetries are statements of a purely algebraic and geometric character, yet when they apply to the dynamics of a system they imply restrictions so powerful that independently of the explicit knowledge of any solution in analytic form (which is often indeed impossible), one nevertheless knows it to be true for a fact that there exists a collection of conserved quantities in direct correspondence with each of the independent symmetry generators of the Lie group. To each of the Lie group generated symmetries, parametrised by the variable α_a, there corresponds a conserved charge, γ^a, the Noether charge. This fundamental result gives a profound insight into the very reason for the possibility of conserved quantities. Furthermore as is discussed hereafter, the expressions for the Noether charges γ^a readily extend to phase space and the Hamiltonian formulation of the dynamics. Within that framework, it turns out that the Noether charges possess an algebra of Poisson brackets such

[18] Again, in the case of a rotational symmetry in space, say, these parameters would correspond to the angles parametrising any such rotation.

that, on the one hand this algebra is isomorphic to the abstract algebra of Lie brackets of the Lie symmetry group G of which they are the conserved charges, and on the other hand, the Noether charges generate through their Poisson brackets with phase space observables the infinitesimal (or linearised) symmetry transformations of the phase space coordinates and observables under the (connected component of the) Lie symmetry group G. From that point of view, and as already mentioned earlier, when a quantisation of the system preserves the structure of the algebra of Noether charges the same conclusions extend to the Hilbert space of quantum states, with in particular conservation of the Noether charges. Quantum states may then be classified in terms of linear representations of the symmetry group G. Their eigenvalues for a maximal abelian subgroup of G (namely, a subset of which all Noether charges commute with one another and may thus be diagonalised simultaneously) then define conserved **quantum numbers** for the quantised system. As an example the conservation of the electric charge immediately comes to mind. Indeed in that case the electric charge is but the Noether charge associated to the U(1) phase symmetry of the electromagnetic interaction. As we know this symmetry is not only a global one, hence leading to a Noether charge which is the electric charge that matter degrees of freedom carry when they couple to the electromagnetic field, but is also a local gauged symmetry with further consequences.

As mentioned already in the case of a local Lie symmetry group, further statements following from the fundamental identity (382) imply two more Noether theorems. One of the consequences of these additional theorems is then that given any solution to the Euler–Lagrange equations of motion, some of which are actually constraint equations rather than genuine dynamical equations of motion, the Noether charges γ^a are not only conserved but vanish identically, $\gamma^a = 0$. Indeed any such solution should thus also be gauge invariant, namely not transform at all under the symmetry, which is possible only provided these charges all vanish. Such configurations, within the context of gauge invariant dynamics, are called **physical configurations** or **physical states**. In the case of the electromagnetic interaction, this condition would translate in an identically vanishing total electric charge of a physical system interacting with the electromagnetic field, thus including also the latter which extends through all of space and time.

5.4 The Noether charge algebra

Given the expression for the Noether charges,

$$\gamma^a = \phi^{an}\,\frac{\partial L}{\partial \dot{q}^n} \,-\, \chi^a\left(\dot{q}^n \frac{\partial L}{\partial \dot{q}^n} \,-\, L\right) \,-\, \Lambda^a, \tag{393}$$

it is clear that these quantities are readily defined over phase space as the following observables,

$$\gamma^a(q^n, p_n) = \phi^{an}(q^n, t) p_n - \chi^a(t)\, H_0(q^n, p_n) \,-\, \Lambda^a(q^n, t), \tag{394}$$

where $H_0(q^n, p_n) = \dot{q}^n\, p_n - L(q^n, \dot{q}^n)$ is the canonical Hamiltonian. Note that even though for a given solution to the equations of motion (whether in Lagrangian or Hamiltonian form) these quantities are conserved with a time independent value, their kinematical expression as phase space observables may carry an explicit time dependence through the functions $\chi^a(t)$, $\phi^{an}(q^n, t)$ and $\Lambda^a(q^n, t)$, depending on the Lie symmetry group G under consideration.

Given this observation, the immediate question which arises is to determine the algebra of Poisson brackets of the Noether charges over phase space. It is indeed possible to give an explicit answer to that question through a careful analysis of the consequences following from the fundamental identity (382) within the Hamiltonian framework. The details of the argument are not discussed in these notes.

In order to describe the result for the algebra of Poisson brackets of the Noether charges, let us first consider the abstract Lie symmetry group G and the algebra of its abstract generators T^a. Being a continuous Lie group of transformations, any of its elements in the component connected to the identity transformation may be written as

$$g[\alpha] = e^{i\alpha_a\, T^a}, \tag{395}$$

α_a being the coordinate parameters of the Lie group as a differential manifold, and T^a the abstract generators of the Lie algebra associated to the Lie group G. The presence of the factor i is a physicist's convention, since within a quantum context one needs such transformations to be also unitary ones in order to preserve quantum probabilities of quantum states under the symmetry transformations, hence one needs

self-adjoint generators T^a if that factor i is included, $T^{a\dagger} = T^a$. Now, given the group composition rules for group elements $g[\alpha]$ and $g[\beta]$, it follows that for the linearised or infinitesimal form of these group transformations, the algebra of generators T^a must possess Lie brackets of the form[19]

$$[T^a, T^b] = iC^{ab}{}_c\, T^c, \tag{396}$$

where the constant coefficients $C^{ab}{}_c$ (the summation convention is again implicit) are known as **the structure constants** or structure coefficients of the Lie algebra of the Lie group G. In the case of a compact Lie group G, such as SU(2) or more generally the unitary groups SU(N), these structure coefficients are real numbers. Note that they are also antisymmetric in their first two indices. Again in the case of compact simple semi-simple compact Lie groups, by introducing the positive definite Killing form on the algebra which then defines an hermitian metric on that vector space, it becomes possible to raise and lower the indices a, b, c (which transform in the adjoint representation of the algebra and group), in which case the structure coefficients C^{abc} or C_{abc} are totally antisymmetric in all three indices.

As an illustration, consider the group[20] SO(3) of all orientation preserving rotations in three dimensional Euclidean space. Rather than using for instance the Euler angle parametrisation of that group, it should be clear that any element of G =SO(3) may be obtained through the composition of the three independent rotations around the three cartesian coordinate axes x^i $(i = 1, 2, 3)$ with an arbitrary angle θ_i in the range $0 \leq \theta_i \leq 2\pi$. Any such transformation thus corresponds to an element of the form

$$g_i[\theta_i] = e^{i\theta_i\, T^i} \qquad \text{[no summation over the index } i\text{]} \tag{397}$$

with a generator T^i (the index i is not summed over in this expression). In order to identify the algebra of SO(3), let us use the defining representation of SO(3) in terms of 3×3 orthogonal matrices of unit determinant acting on three component vectors. It is well known how the matrix representations of each of the above elements $g_i[\theta_i]$ are expressed, for example for the rotation of angle θ_3 around the third axis $i = 3$,

$$g_3[\theta_3] : \qquad \begin{pmatrix} \cos\theta_3 & \sin\theta_3 & 0 \\ -\sin\theta_3 & \cos\theta_3 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{398}$$

Expanding such expressions to first order in the angles θ_i, the matrix representations of the generators T^i are readily identified through $g_i[\theta_i] = \mathbb{I} + i\theta_i T^i + \cdots$, leading to the following matrix elements

$$\left(T^i\right)^j{}_k = -i\epsilon^{ijk}, \qquad i, j, k = 1, 2, 3, \tag{399}$$

ϵ^{ijk} being the usual totally antisymmetric invariant tensor in three dimensional Euclidean space, with $\epsilon^{123} = +1$. Simple matrix multiplication then finds that the algebra of commutators of these SO(3) generators, defining the Lie brackets of the abstract Lie algebra $so(3)$ of the finite compact Lie group SO(3), is

$$\left[T^i, T^j\right] = i\,\epsilon^{ijk}\, T^k, \tag{400}$$

where the summation of the repeated index k is implicit and to be understood. Hence the structure constants of the Lie algebra $so(3)$ are indeed real and totally antisymmetric structure coefficients, given by the antisymmetric tensor ϵ^{ijk}. It is left as an exercise for the reader to repeat the analysis for the compact Lie group SU(2) of unitary 2×2 matrices of unit determinant over the complex numbers, to discover that the algebra $su(2)$ of that Lie group in fact coincides with that of $so(3)$, $su(2) = so(3)$. Incidentally, this is precisely what has been observed when finding the symmetry reason behind the degeneracies of the energy spectrum of the two dimensional spherically symmetric harmonic oscillator. This equivalence between a unitary group Lie algebra, $su(2)$, and an orthogonal group Lie algebra, $so(3)$, is specific to this particular case.

[19] A Lie algebra is defined in terms of a Lie bracket, in a manner similar to that in which a phase space is defined in terms of Poisson brackets. For all practical purposes in these notes one may think of the Lie bracket as the ordinary commutator of abstract operators, or even matrices, since one is implicitly interested in Hilbert space realisations of the abstract Lie group symmetry and its algebra.

[20] The reader is invited to consider the case of rotations in the two dimensional plane with symmetry group SO(2), and derive the same considerations, to conclude that the algebra is that of the group U(1) of phase transformations in the complex plane, with a single generator hence an abelian algebra and thus a vanishing structure constant.

Having thus introduced the concepts of generators and structure constants of the Lie algebra associated to a Lie symmetry group, let us consider the issue of the Poisson brackets of the Noether charges γ^a. First, in the case that no total time derivative term $\Lambda(q^n, t)$ is induced in the action through the symmetry transformation, it may be shown that the algebra of these Poisson brackets is always given as

$$\{\gamma^a, \gamma^b\} = C^{ab}{}_c \, \gamma^c \tag{401}$$

(the summation convention is implicit), precisely in terms of the structure constants $C^{ab}{}_c$ of the Lie algebra of the symmetry group G. Except for a factor i which may easily be introduced by considering the Poisson brackets of the pure imaginary quantities $i\gamma^a$, this algebra of Poisson brackets thus coincides with the Lie bracket of the abstract Lie algebra of G. Note that at the quantum level, through the correspondence principle, the Noether charge operators $\hat{\gamma}^a$ should then obey the algebra of commutation relations

$$[\hat{\gamma}^a, \hat{\gamma}^b] = i\hbar C^{ab}{}_c \, \hat{\gamma}^c, \qquad (\hat{\gamma}^a)^\dagger = \hat{\gamma}^a, \tag{402}$$

if the symmetry is to be realised in the quantised system as well (operator ordering issues are at play here and one has to identify a quantisation which preserves these commutation relations while also producing self-adjoint Noether charges $\hat{\gamma}^a$). Except for the factor $\hbar$ which is easily absorbed through a rescaling of the Noether charges, $\hat{\gamma}^a/\hbar$, one then has identically the algebra of the abstract Lie algebra, realised in terms of the quantum observables $\hat{\gamma}^a/\hbar$ on the Hilbert space of the quantised system. In particular, this implies that finite Lie symmetry group transformations are realised on the Hilbert space of quantum states by the unitary operators

$$e^{\frac{i}{\hbar}\alpha_a \hat{\gamma}^a}, \tag{403}$$

defined in terms of the properly normalised Noether charge operators $\frac{1}{\hbar}\hat{\gamma}^a$.

These results thus establish that indeed the Noether charges, as conserved quantities the existence of which follows from the symmetries, are also the generators of these symmetries, either on phase space through their Poisson brackets with the phase space coordinates and other observables in the classical context, or on Hilbert space through their action on quantum states as quantum operators. Conserved charges are the generators of the symmetries of which they are the Noether charges. In particular at the quantum level, selecting a maximal subset of Noether charges which all commute with one another, namely a maximal abelian subalgebra, all these operators may be diagonalised simultaneously, thereby leading to a basis of states of Hilbert space each of which element carries specific conserved quantum charges under the symmetry, namely the associated eigenvalues under the symmetries of one of its maximal abelian subgroups. For instance returning to the example of SO(3), any maximal abelian subalgebra of $so(3)$ is one dimensional. Taking for instance the subalgebra generated by T^3, namely rotations around the axis $i = 3$, quantum states are then classified in terms of their charge under T^3, namely their angular-momentum component along the axis $i = 3$ in units of $\hbar$. Because of the structure of representations of $so(3) = su(2)$ labelled by the integer or half-integer spin value j as already discussed in the context of the two dimensional spherically symmetric harmonic oscillator, these components of angular-momentum for an arbitrary system are quantised in the range $-j \leq m \leq j$ in integer steps for the eigenvalues m of T^3.

Since there are examples of symmetries of physical relevance which induce a total time derivative in the action, let us now describe the general result. Though not necessarily always the case, it may then happen that the algebra of Poisson brackets of the Noether charges is no longer of the form (401) but acquires an extra contribution through one extra term independent of time and the phase space variables, a so-called central extension of the Lie algebra of G since this extra contribution has vanishing Poisson brackets or quantum commutation relations with all elements of the algebra of observables of the system, whether classical or quantised. Namely one has in general the expression

$$\{\gamma^a, \gamma^b\} = C^{ab}{}_c \, \gamma^c + C^{ab}, \tag{404}$$

where the antisymmetric constant coefficients C^{ab} are obtained as follows. Under the group composition law, one has a certain composition law for the group parameters α_a, namely,

$$g[\alpha] \, g[\beta] = g[\eta(\alpha, \beta)]. \tag{405}$$

As a matter of fact, the structure coefficients of the Lie algebra of G are given as follows from the functions $\eta_a(\alpha, \beta)$,

$$\frac{\partial^2}{\partial\alpha_a \partial\beta_b} \left[\eta_c(\alpha, \beta) - \eta_c(\beta, \alpha)\right]_{|_{\alpha=0=\beta}} = C^{ab}{}_c. \tag{406}$$

By considering then how the Lagrange function transforms under such a composition of symmetry transformations it may be shown that one has necessarily,

$$\Lambda\left(q^n,t;\gamma(\alpha,\beta)\right)\,-\,\Lambda\left(q^{n\prime}(q^n,t;\beta),t'(t;\beta);\alpha\right)\,-\,\Lambda\left(q^n,t;\beta\right)=C\left(\alpha,\beta\right), \tag{407}$$

where $C(\alpha,\beta)$ are thus specific functions of the group parameters, in fact associated to cocycle properties of the symmetry group encoded through the function $\Lambda(q^n,t;\alpha)$. The quantities C^{ab} appearing in the above general Poisson brackets of the Noether charges are then given as

$$C^{ab}=\frac{\partial^2}{\partial\alpha_a\partial\beta_b}\left[C(\alpha,\beta)\,-\,C(\beta,\alpha)\right]_{|_{\alpha=0=\beta}}. \tag{408}$$

Incidentally, it may easily be checked that a redefinition of the Lagrange function by a total time derivative, thus leaving the equations of motion invariant, does not modify these central extension coefficients C^{ab}.

What is interesting about this result is that central extensions are often believed to arise only at the quantum level, and to correspond then to an explicit breakdown of the classical symmetry generated by the Noether charges, a phenomenon called **a quantum anomaly**. Here we see that classical extensions are also possible, provided the action varies under a symmetry with a total time derivative which itself must possess some nontrivial cocycle property, as a consequence of some nontrivial topology properties in the configuration space of the system. Examples are described hereafter. At the quantum level, the symmetry is then realised not through a faithful representation of the symmetry group (the type of representation encountered so far in terms simply of the action of $\exp\left(\frac{i}{\hbar}\alpha\hat{\gamma}^a\right)$), but in terms of what is called **a projective representation** of the abstract Lie symmetry group such that symmetry transformations of quantum states are obtained not only through the action of the unitary operators $e^{\frac{i}{\hbar}\alpha_a\hat{\gamma}^a}$ but also some further phase factor which is function of the group parameters α_a and in direct correspondence with the total time derivative contribution $\Lambda(q^n,t;\alpha)$ (as may heuristically be understood from the path integral representation of quantum physics). Even though we shall not make use later on of such features specific to certain classes of Lie group symmetries, it is important to know about the existence of such particular situations and the possibility of classical central extensions of Lie algebras in the classical Poisson bracket algebra of Noether charges.

Remark

One final remark concerning symmetries and their Noether charges may be made in order to conclude this discussion. The result (392) gives the general expression for these charges in terms of the functions parametrising the linearised variations of t, q^n and the induced total time derivative term Λ under the symmetry group G. However, in practice and in almost all cases (except for field theories of supergravity to the best of this author's knowledge) one may rather easily identify the Noether charges through the following little trick. In the case that the symmetry parameters α_a are constant, the action is invariant up to a total time derivative term,

$$S[q^{n\prime}]=S[q^n]+\int dt\ \text{t.t.d.}, \tag{409}$$

where "t.t.d." stands for some unspecified total time derivative contribution. In the case of a linearised or infinitesimal symmetry transformation, one thus has

$$\delta S[q^n]=\int dt\ \text{t.t.d.}\ . \tag{410}$$

Imagine now for the sake of the argument that the symmetry transformation is considered for parameters $\alpha_a(t)$ which are arbitrary functions of time. Except when in fact the symmetry is a local gauge symmetry, the action may then no longer change just by a total time derivative, since it is then no longer invariant up to such a term. Rather in general it is expected then not to be invariant up to such terms, but to vary by terms involving the first order time derivative of the symmetry parameters $\alpha_a(t)$ since the Lagrange function is function of both $q^n(t)$ and $\dot{q}^n(t)$. Hence we should expect a linearised variation of the form

$$\delta S[q^n]=\int dt\,\left[\frac{d\alpha_a}{dt}\,Q^a\,+\,\text{t.t.d.}\right], \tag{411}$$

where $Q^a(q^n, \dot{q}^n, t)$ are some quantities which could *a priori* be functions of the generalised coordinates and their velocities as well as time. Clearly when the parameters $\alpha_a(t)$ are constants one recovers the symmetry property of the action. In the latter form one may now integrate by parts and bring that variation of the action into the form

$$\delta S[q^n] = \int dt \, \left[-\alpha_a \, \frac{dQ^a}{dt} \, + \, \text{t.t.d.} \right]. \tag{412}$$

However, since when the parameters $\alpha_a(t)$ are constants the action may only change by a total time derivative, one must conclude that the quantities Q^a must be conserved quantities, $dQ^a/dt = 0$. In other words, possibly up to an overal sign, necessarily the quantities $Q^a(q^n, \dot{q}^n, t)$ must coincide with the Noether charges $\gamma^a(q^n, \dot{q}^n, t)$ associated to the symmetry leaving the action invariant up to total time derivatives, which are in fact readily defined over the phase space of the system. This method is quite generally sufficient in order to readily identify the Noether charges given a symmetry of the action, rather than going through the identification of the functions $\chi^a(t)$, $\phi^{an}(q^n, t)$ and $\Lambda^a(q^n, t)$ introduced in the above general discussion of Noether's first theorem.

5.5 Illustrations

5.5.1 Time translation invariance

As an illustration of the general discussion of Noether's first theorem, let us begin by considering any dynamical system described by an action of the type we have been using ever since the beginning of these notes,

$$S[q^n] = \int dt \, L(q^n, \dot{q}^n). \tag{413}$$

Having excluded from the outset any explicit time dependence of the Lagrange function, it is quite obvious that this dynamics is invariant under arbitrary constant translations in the time variable t. Any transformation of the form

$$t' = t + t_0, \qquad q^{n\prime}(t') = q^n(t), \tag{414}$$

defines an invariance of the action, with no total time derivative term being induced, $\Lambda(q^n, t) = 0$, simply because we have all along assumed the Lagrange function not to possess any explicit time dependence. This group of symmetries is a one dimensional Lie group with as continuous parameter the constant quantity t_0 defining the translation in time. There thus exists a conserved charged associated to time translation invariance in the evolution parameter t used to parametrise the dynamics of the system.

For what concerns then linearised or infinitesimal transformations, the index a of the variables α_a of the general discussion takes only a single value in the present case, $a = 1$. Furthermore, one readily identifies

$$\chi^a(t) = 1, \qquad \phi^{an}(q^n, t) = 0, \qquad \Lambda^a(q^n, t) = 0. \tag{415}$$

By direct substitution into the definition (392) of the Noether charges, one finds that the Noether charge associated to this symmetry is

$$\gamma^a = - \left[\dot{q}^n \, \frac{\partial L}{\partial \dot{q}^n} \, - \, L \right] = - \, H_0(q^n, p_n). \tag{416}$$

Hence in full generality, whenever a system is invariant under translations in its time evolution parameter, its canonical Hamiltonian is a conserved quantity, a constant of motion which coincides with the Noether charge for that symmetry. Furthermore, this Noether charge indeed does generate infinitesimal translations in the time evolution parameter, namely it is the generator of the time dependence of the system through the Poisson brackets. This latter fact is an explicit illustration of the general result that Noether charges are the generators of the symmetries of which they are the conserved quantities.

This conclusion applies likewise at the quantum level as may easily be seen. Let us consider an orthonormalised basis of Hilbert space consisting of the energy eigenstates $|E_m\rangle$ where, in keeping with our previous generic notation, in general m stands for a multi-index some of which components could even

take values in a continuous range. As we know the exponentiated action of the quantum Hamiltonian on quantum states generates their time evolution,

$$|\psi, t\rangle = e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}\,|\psi, t_0\rangle = \sum_m |E_m\rangle\, e^{-\frac{i}{\hbar}(t-t_0)E_m}\,\langle E_m|\psi, t_0\rangle, \tag{417}$$

which shows indeed that the quantum Hamiltonian is the generator of constant translations in time, in the present case by the value $(t - t_0)$ for the quantum evolution operator $U(t, t_0) = e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}$.

Note that the time evolution parameter does not, in general, necessarily coincide with the physical time, when one considers parametrised systems such as the relativistic particle, string theory and general relativity. However, when the time evolution parameter coincides with the physical time, the above conservation law shows that in direct correspondence with the invariance of a dynamics under arbitrary time translations its total energy is a conserved quantity, namely the Noether charge generating that symmetry.

5.5.2 Nonrelativistic particles

In order to display other examples of direct relevance even to nonrelativistic Newton dynamics, we now consider systems of nonrelativistic particles in interaction through some conservative forces in different situations, and then identify each of the conservation laws of mechanical energy, momentum and angular-momentum. Consider a system of N particles of masses m_α $(\alpha = 1, 2, \ldots, N)$, of position vectors $\vec{r}_\alpha(t)$ with respect to some inertial frame, and subjected to conservative forces of total potential energy $V(\vec{r}_\alpha - \vec{r}_\beta)$, namely some function of pairwise differences of the position vectors. As is well known the Lagrange function for such a system is

$$L(\vec{r}_\alpha, \dot{\vec{r}}_\alpha) = \sum_{\alpha=1}^{N} \frac{1}{2} m_\alpha \dot{\vec{r}}_\alpha{}^2 \; - \; V(\vec{r}_\alpha - \vec{r}_\beta). \tag{418}$$

For later purposes, the cartesian coordinates of the particles will be denoted x^i_α with $i = 1, 2, 3$ in three dimensional Euclidean space. These are the configuration space degrees of freedom of the system, the index n of the general discussion standing here for the double index (i, α) taking $3N$ values.

Time translation invariance

From the previous example in the general case, at once we know that the canonical Hamiltonian of this system is the Noether charge for time translation invariance of this system, since the Lagrange function does not possess any explicit time dependence (this would thus no longer be the case had the particles been coupled to a time dependent background electromagnetic field $\vec{E}(t, \vec{r}\,)$ and $\vec{B}(t, \vec{r}\,)$, as was already established explicitly earlier in these notes). Since the time evolution parameter t of the system is also the physical time, we conclude that the total mechanical energy of the system, namely its canonical Hamiltonian,

$$H_0 = \sum_{\alpha=1}^{N} \frac{1}{2m_\alpha} \vec{p}_\alpha{}^2 \; + \; V(\vec{r}_\alpha - \vec{r}_\beta), \tag{419}$$

is the conserved Noether charge generating infinitesimal time translations.

Space translation invariance

Given that the total potential energy is taken to be function only of the pairwise differences in the position vectors of the particles, the system is also invariant under arbitrary constant translations in space, namely

$$t' = t, \qquad \vec{r}\,'_\alpha(t') = \vec{r}_\alpha(t) + \vec{r}_0. \tag{420}$$

These transformations do not induce any total time derivative term in the action, $\Lambda(\vec{r}_\alpha, t) = 0$. The continuous parameters of this Lie symmetry group are the three cartesian components of the translation vector, $\vec{r}_0 = (r_{0,a})$, distinguished by the label $a = 1, 2, 3$ in order to use the notations of the general

discussion and avoid any confusion with the cartesian index i of the coordinates x^i_α. When linearised in the parameters $r_{0,a}$, the above transformations imply

$$\chi^a(t) = 0, \qquad \phi^{ai}_\alpha(\vec{r}_\alpha, t) = \delta^{ai}, \qquad \Lambda^a(\vec{r}_\alpha, t) = 0. \tag{421}$$

Consequently, using the general definition (392), the Noether charges generating the space translation invariance of the system are

$$\gamma^a = \sum_{\alpha=1}^{N} \sum_{i=1}^{3} \phi^{ai}_\alpha \, p_{\alpha,i} = \sum_{\alpha=1}^{N} p^a_\alpha, \tag{422}$$

where $p^a_\alpha = m\dot{x}^a_\alpha$ are the conjugate momenta of the coordinates x^a_α, namely the cartesian components of the momentum of particle α.

In conclusion, the Noether charges related to invariance under translations in space are the components of the total momentum vector of the system of particles,

$$\vec{\gamma} = \sum_{\alpha=1}^{N} \vec{p}_\alpha = \vec{P}. \tag{423}$$

Again this is a most general result valid for any system invariant under space translations.

This conclusion remains also valid at the quantum level. For the sake of pointing this out explicitly, let us restrict to a single degree of freedom system of cartesian coordinate $x(t)$ with $p(t)$ as its conjugate momentum. At the quantum level the operators $\hat{x}$ and $\hat{p}$ obey the Heisenberg algebra, $[\hat{x}, \hat{p}] = i\hbar$. Considering for instance the configuration space representation in terms of configuration space wave functions $\psi(x) = \langle x|\psi\rangle$, $|x\rangle$ being the normalised position eigenstates, we know that the momentum operator is represented as,

$$\hat{p}: \qquad -i\hbar \frac{d}{dx}\psi(x). \tag{424}$$

In other words, we have,

$$\frac{i}{\hbar}\hat{p}: \qquad \frac{d}{dx}\psi(x). \tag{425}$$

That this differential operator is indeed the generator for infinitesimal translations in space follows from the Taylor series expansion

$$\psi(x+a) = \psi(x) + a\frac{d\psi(x)}{dx} + \frac{1}{2!}a^2\frac{d^2\psi(x)}{dx^2} + \cdots = \sum_{n=0}^{\infty} \frac{1}{n!} a^n \frac{d^n\psi(x)}{dx^n} = e^{a\frac{d}{dx}}\,\psi(x) = e^{\frac{i}{\hbar}a\hat{p}}\,\psi(x). \tag{426}$$

An alternative way of seeing this result without relying on the wave function representation is by considering the following action of the exponentiated operator $\hat{p}$,

$$e^{-\frac{i}{\hbar}a\,\hat{p}}\,|x\rangle. \tag{427}$$

In order to identify which quantum state is obtained, let us act on it with the position operator $\hat{x}$ and use one of the Baker–Campbell–Hausdorff formulae,

$$\begin{aligned}
\hat{x}\,e^{-\frac{i}{\hbar}a\hat{p}}\,|x\rangle &= e^{-\frac{i}{\hbar}a\hat{p}}\,e^{\frac{i}{\hbar}a\hat{p}}\,\hat{x}\,e^{-\frac{i}{\hbar}a\hat{p}}|x\rangle \\
&= e^{-\frac{i}{\hbar}a\hat{p}}\left(\hat{x} + \left[\frac{i}{\hbar}a\hat{p}, \hat{x}\right]\right)\,|x\rangle \\
&= e^{-\frac{i}{\hbar}a\hat{p}}\,(x+a)\,|x\rangle \\
&= (x+a)\,e^{-\frac{i}{\hbar}a\hat{p}}\,|x\rangle.
\end{aligned} \tag{428}$$

In other words, the state obtained by the action of $e^{-\frac{i}{\hbar}a\hat{p}}$ on $|x\rangle$ is necessarily proportional to the position eigenstate $|x+a\rangle$. In order to identify the corresponding coefficient or component, we need only project it onto any of the position eigenstate basis vectors $|x'\rangle$,

$$\begin{aligned}
\langle x'|e^{-\frac{i}{\hbar}a\hat{p}}|x\rangle &= \int_{-\infty}^{+\infty} dp\,\langle x'|e^{-\frac{i}{\hbar}a\hat{p}}|p\rangle\langle p|x\rangle \\
&= \int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar}\,e^{\frac{i}{\hbar}(x'-x-a)p} \\
&= \delta\left(x' - (x+a)\right).
\end{aligned} \tag{429}$$

In other words, we have

$$e^{-\frac{i}{\hbar}a\,\hat{p}}\,|x\rangle = |x+a\rangle. \tag{430}$$

From this it also follows that we have for any state $|\psi\rangle$,

$$\langle x|e^{\frac{i}{\hbar}a\,\hat{p}}|\psi\rangle = \langle x+a|\psi\rangle = \psi(x+a). \tag{431}$$

Hence indeed the exponentiation $e^{\frac{i}{\hbar}a\hat{p}}$ of the conjugate momentum operator $\hat{p}$ generates a finite translation by the value a in the configuration space coordinate x, while $\frac{i}{\hbar}\hat{p}$ is the generator of infinitesimal translations in x. Incidentally, the very last of these relations may also be used as a starting point to establish the functional representations of the quantum operators $\hat{x}$ and $\hat{p}$ in the configuration space wave function representation of the Hilbert space realising the Heisenberg algebra.

Space rotation invariance

In order to address the consequences of invariance under space rotations, let us now furthermore assume that the total potential energy is function only of the pairwise distances $|\vec{r}_\alpha - \vec{r}_\beta|$ between the particles, $V(|\vec{r}_\alpha - \vec{r}_\beta|)$. Clearly in such a situation the action is invariant under arbitrary constant rotations of the position vectors, namely with

$$t' = t, \qquad \vec{r}\,'_\alpha(t) = R\cdot\vec{r}_\alpha(t), \qquad \Lambda(\vec{r}_\alpha, t) = 0, \tag{432}$$

where R stands for the rotation matrix acting on the components of each of the position vectors $\vec{r}_\alpha$. The parameters of the corresponding Lie symmetry group are three independent and continuous rotation angles. Using the previous discussion for such transformations with as generators those that generate rotations of angle θ_a around the axis $a = 1, 2, 3$, namely the matrices $(T^a)^j{}_k = -i\epsilon^{ajk}$ constructed above, the linearised form of these symmetry transformations is

$$\delta t(t) = 0, \qquad \delta x^i_\alpha = i\theta_a (T^a)^i{}_j\, x^j_\alpha, \qquad \delta\Lambda(\vec{r}_\alpha, t) = 0. \tag{433}$$

Consequently we identify

$$\chi^a(t) = 0, \qquad \phi^{ai}_\alpha(\vec{r}_\alpha, t) = \epsilon^{aij}\, x^j_\alpha, \qquad \Lambda^a(\vec{r}_\alpha, t) = 0. \tag{434}$$

By substitution into (392) the associated Noether charges are

$$\gamma^a = \sum_{\alpha=1}^{N}\sum_{i=1}^{3} \epsilon^{aij}\, x^i_\alpha\, p_{\alpha,j}. \tag{435}$$

In other words, the Noether charges which generate space rotation invariance are the components of the total angular-momentum vector of the system,

$$\vec{\gamma} = \sum_{\alpha=1}^{N} \vec{r}_\alpha \times \vec{p}_\alpha = \vec{L}. \tag{436}$$

Once again this result is most general and applies to any system invariant under constant rotations in space.

It thus is quite remarkable that symmetry properties of space and time, in the present case the symmetries of three and one dimensional Euclidean space and time, when also shared by the dynamics of a system, imply the existence of conserved quantities whatever the configuration of the system solving its equations of motion. These conserved quantities are also the generators of these symmetries on phase space through the Poisson brackets of these conserved quantities with any phase space observable, beginning with the phase space coordinates. Indeed, within the Hamiltonian framework it readily follows that the above Noether charges do generate the corresponding infinitesimal symmetry transformations of the configuration space coordinates, while their Poisson brackets are isomorphic to the Lie algebra of the Lie symmetry group of which they are the Noether charges. In particular the Poisson brackets of the total momentum $\vec{P}$ and angular-momentum $\vec{L}$ components with the generator of time translations are

$$\big\{H, P^i\big\} = 0, \qquad \big\{H, L^i\big\} = 0, \tag{437}$$

indeed expressing the conservation of these quantities, whereas among themselves they possess the Poisson brackets,

$$\begin{aligned} \left\{P^i, P^j\right\} &= 0, \\ \left\{L^i, P^j\right\} &= \epsilon^{ijk}\, P^k, \\ \left\{L^i, L^j\right\} &= \epsilon^{ijk}\, L^k \end{aligned} \tag{438}$$

(summation over repeated indices is implicit). This algebra is recognised to be that of the Euclidean group $E(3)$ in three dimensional Euclidean space. The first set of brackets represents the fact that any two translations commute with one another, whereas the last two sets of brackets represent the fact that under space rotations the vector generator of translations transforms as a vector quantity, and likewise for the vector generator of space rotations. Note also that the algebra of the angular-momentum coincides with the abstract $so(3)$ algebra constructed previously. This also implies that at the quantum level, this algebra will be realised in the space of quantum states in terms of their spin values in the manner already discussed.

5.5.3 The free nonrelativistic particle

Now as an illustration of a symmetry leading to a central extension in the algebra of Poisson brackets of its Noether charges, consider a single free nonrelativistic particle in Euclidean space,

$$L = \frac{1}{2} m \dot{\vec{q}}^2, \qquad H_0 = \frac{1}{2m}\, \vec{p}^{\,2}. \tag{439}$$

Besides the symmetries discussed above, Newton's mechanics is known to be invariant under Galilei boosts, namely a six dimensional Lie symmetry group, with

$$t' = t, \qquad \vec{q}\,'(t') = \vec{q}(t) \,+\, \vec{a} \,+\, \vec{V}\, t, \tag{440}$$

$$L' = L + m\, \vec{V} \cdot \dot{\vec{q}} + \frac{1}{2} m \vec{V}^{\,2}, \qquad \Lambda\left(\vec{q}, t; \vec{a}, \vec{V}\right) = m\, \vec{V} \cdot \vec{q} + \frac{1}{2} m\, \vec{V}^{\,2}\, t. \tag{441}$$

Hence even though the simplest of systems, a total time derivative is induced in the action under Galilei boosts, namely space translations which are no longer constant but linear in time, or of constant velocity, bringing the system from one inertial frame to another with the relative velocity $\vec{V}$.

Then, with indices a, b in correspondence with the continuous Lie group parameters through $a, b \leftrightarrow \left(\vec{a}, \vec{V}\right) = \left(a^i, V^i\right)$ and $i = 1, 2, 3$ labelling vector components, it readily follows that the coefficients $C(\alpha, \beta)$ of the general discussion as well as the central extension constants C^{ab} are given as,

$$C\left(\vec{a}_1, \vec{V}_1; \vec{a}_2, \vec{V}_2\right) = -m\, \vec{V}_1 \cdot \vec{a}_2, \qquad C^{ab} = \begin{pmatrix} 0 & m\mathbb{I} \\ -m\mathbb{I} & 0 \end{pmatrix}. \tag{442}$$

Identifying then all the relevant quantities which enter the definition (392), the Noether charges are found to be

$$\gamma^a = \left(p^i, \gamma^i\right), \qquad p^i = m\dot{q}^i, \qquad \gamma^i = p^i\, t \,-\, m q^i, \tag{443}$$

with the Noether algebra

$$\left\{p^i, p^j\right\} = 0, \quad \left\{p^i, \gamma^j\right\} = m\, \delta^{ij}, \quad \left\{\gamma^i, p^j\right\} = -m\, \delta^{ij}, \quad \left\{\gamma^i, \gamma^j\right\} = 0, \tag{444}$$

namely

$$\left\{\gamma^a, \gamma^b\right\} = C^{ab}. \tag{445}$$

Hence indeed, the generators $\vec{\gamma} = \vec{p}\, t - m\vec{q}$ of Galilei boosts have a Poisson algebra with a central extension term which is the mass of the particle. Such a parameter does not appear in the abstract algebra of the Galilei group, simply because no such physical parameter is then available. But in the present system this symmetry is realised even though with a central extension determined by the unique physical parameter available, the mass m of the free nonrelativistic particle.

Note than in spite of the explicit time dependence appearing in the definition of the vector Noether charge generating Galilei boosts, this quantity is conserved nonetheless. Indeed, the Hamiltonian equations of motion for the above Noether charges are

$$\frac{dp^i}{dt} = \left\{p^i, H_0\right\} = 0, \qquad \frac{d\gamma^i}{dt} = \frac{\partial \gamma^i}{\partial t} + \left\{\gamma^i, H_0\right\} = p^i - p^i = 0, \tag{446}$$

yet

$$\left\{\gamma^i, H_0\right\} = -p^i \neq 0 \tag{447}$$

since $\partial\gamma^i/\partial t = p^i \neq 0$. At the quantum level within the Heisenberg picture of quantum physics, the Schrödinger equation for the quantum operator $\hat{\vec{\gamma}}$ generating Galilei boosts has to be adapted accordingly, to account for the explicit time dependence of that operator,

$$\hat{\gamma}(t) = \hat{p}(t_0)\, t - m\hat{\vec{q}}(t). \tag{448}$$

For an arbitrary quantum operator $\hat{A}$ which may have in a likewise manner an explicit time dependence, this extension of the Schrödinger equation in the Heisenberg picture reads,

$$i\hbar\frac{d\hat{A}}{dt} = i\hbar\frac{\partial \hat{A}}{\partial t} + \left[\hat{A}, \hat{H}_0\right]. \tag{449}$$

5.5.4 The free extended Landau problem

As a final illustration of interest, let us consider a charged particle confined to the two dimensional Euclidean plane and subjected to static and homogeneous magnetic and electric fields, $\vec{B}$ and $\vec{E}$, the former perpendicular to the plane and the latter lying within it. In the symmetric gauge this system is described by the Lagrange function

$$L = \frac{1}{2}m\delta_{ij}\,\dot{x}^i\dot{x}^j - \frac{1}{2}qB\,\epsilon_{ij}\,\dot{x}^i x^j + q\,x^i E_i, \qquad \epsilon_{12} = \epsilon^{12} = +1, \quad i,j = 1,2. \tag{450}$$

Clearly such a system is invariant under arbitrary translations in the plane, forming a two parameter abelian Lie group of symmetries. Yet, the action is not invariant, but transforms by a total time derivative,

$$t' = t, \qquad x'^i(t') = x^i(t) + a^i, \tag{451}$$

$$L' = L - \frac{1}{2}qB\,\epsilon_{ij}\dot{x}^i a^j + q\,a^i E_i, \qquad \Lambda\left(\vec{x}, t; \vec{a}\right) = -\frac{1}{2}qB\,\epsilon_{ij}\,x^i a^j + q\,a^i E_i\,t. \tag{452}$$

The associated cocycle function $C(\alpha,\beta)$ of the general discussion is then found to be

$$C\left(\vec{a},\vec{b}\right) = -\frac{1}{2}qB\,\epsilon_{ij}\,a^i b^j, \tag{453}$$

leading to the central extension coefficients

$$C^{ij} = -qB\,\epsilon^{ij}. \tag{454}$$

The Noether charges that follow read

$$\gamma^i = p^i - \frac{1}{2}qB\,\epsilon^{ij}x^j - qE^i\,t, \tag{455}$$

with the algebra

$$\left\{\gamma^i, \gamma^j\right\} = -qB\,\epsilon^{ij} = C^{ij}, \tag{456}$$

and indeed generate translations in the plane as may checked by computing their Poisson brackets with the phase space coordinates x^i and p_i.

Given the canonical Hamiltonian

$$H_0 = \frac{1}{2m}\left[p^i + \frac{1}{2}qB\,\epsilon^{ij}\,x^j\right]^2 - q\,x^i E^i, \tag{457}$$

the Hamiltonian equations of motion of these generators of space translations are

$$\frac{d\gamma^i}{dt} = \frac{\partial\gamma^i}{\partial t} + \{\gamma^i, H_0\} = 0, \tag{458}$$

thus indeed these charges are conserved. Nevertheless, they possess an explicit time dependence,

$$\{\gamma^i, H_0\} = -\frac{\partial\gamma^i}{\partial t} = q\,E^i \neq 0 \tag{459}$$

Remark

It is possible to consider the motion of the magnetic center defined as

$$\vec{C} = \vec{x} + \frac{m}{q|\vec{B}\,|}\,\dot{\vec{x}} \times \vec{B}, \tag{460}$$

namely the instantaneous rotation center of the particle. Using the Lorentz force equation of motion,

$$m\ddot{\vec{x}} = q\,\vec{E} + q\,\dot{\vec{x}} \times \vec{B}, \tag{461}$$

one finds

$$\dot{\vec{C}} = \frac{1}{|\vec{B}\,|}\vec{E} \times \vec{B}. \tag{462}$$

Hence when the electric field $\vec{E}$ is present the magnetic center follows a trajectory of constant velocity in a direction perpendicular to the electric field and given by the vector product $\vec{E} \times \vec{B}$.

6 Conclusions

The main purpose of the present notes has been two-fold. On the one hand, to introduce to the basic concepts and formalism of quantum physics in a language which probably emphasizes more the algebraic and mathematical aspects of that general physics framework than what is usually found in most textbooks or introductory notes on the subject. On the other hand, at the same time to highlight the fundamental rôle of symmetries in physics, and in particular quantum physics, in relation both to Noether's (first) theorem and to the representation theory of symmetry groups. All throughout, the general discussion put within the context of mechanical systems rather than field theories, has been illustrated with rather familiar examples, and yet, examples which already provide very useful insight into what lies in store beyond the contents of these notes. For instance, it has been indicated how among symmetries those that are local, namely the realisation of the principle of gauge invariance, do play a fundamental rôle in the modern theories of the fundamental interactions, be they classical or quantum.

And as a matter of fact the ambition of these notes has been to bring the reader onto the threshold from where he/she may now embark on his/her own into the study of quantum field theories, their relativistic quantum particle interpretation and the perturbative description of their interactions. By extending to the relativistic context the methods and concepts developed in these notes, one quickly comes to the conclusion that relativistic quantum field theories and relativistic quantum particles are just two dual aspects of a common underlying physical reality, that of quantum interactions in a relativistic spacetime of unified matter and radiation phenomena. How this is indeed achieved is discussed in quite many textbooks on Quantum Field Theory, such as in Ref. [4], leading then to the remarkable achievements of perturbative renormalisation theory. However, an introductory exposition to that subject in the spirit of the present notes, and which builds on its contents, may also be found in lectures notes available from other Volumes in the present Proceedings Series [1, 2].

Simply, by having interwoven the mathematics and the physics of quantum physics in the present introductory discussion of the concepts of the quantum world, it is hoped that both our more mathematics or more physics inclined readers will find sufficient inspiration from these notes to launch their own line of study and research into this world of physics at the frontiers of today in both mathematics and physics, in search of a fundamental unification of the conceptual representation of the physical Universe.

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