# Quantum modes

*Ion I. Cotaescu*

# The classical motion

The space of the classical physics is the Euclidean space $E(3)$ where any orthogonal basis $\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ can be associated to the system of Cartesian coordinates $(x^1, x^2, x^3)$ having the origin in a fixed point $O$. In addition, the time $t \in \mathbb{R}^+$ is considered to be universal. Thus, one defines the ***frame*** $(t, x^1, x^2, x^3)$. In this notation the position vector reads $\vec{x} = x^i \vec{e}_i$ ($i, j, k, ... = 1, 2, 3$).

The classical mechanics studies the motion of massive point-wise particles. A particular case is of a particle of mass $m$ moving in an external field of ***conservative*** forces

$$\vec{F}(\vec{x}) = -\mathrm{grad}\, V(\vec{x}) \tag{1}$$

derived from the static potential $V$. Then the trajectory $\vec{x}(t)$ results from the Newton dynamical principle which can be exploited in different formalisms (Newton, Lagrange and Hamilton).

| | Newton | Lagrange | Hamilton |
|---|---|---|---|
| trajectory | $\vec{x}(t) \in E(3)$ | $\vec{x}(t) \in E(3)$ | $\{\vec{x}(t),\, \vec{p}(t)\} \in E(3) \times E_p(3)$ |
| function | | $\mathcal{L}(\vec{x}, \dot{\vec{x}}) = \frac{1}{2}\, m\dot{\vec{x}}^{\,2} - V(\vec{x})$ | $\mathcal{H}(\vec{x}, \vec{p}) = \frac{1}{2m}\, \vec{p}^{\,2} + V(\vec{x})$ |
| momentum | $\vec{p} = m\dot{\vec{x}}$ | $p^i = \frac{\partial \mathcal{L}}{\partial \dot{x}^i}$ | $\dot{\vec{x}} \to \dot{\vec{x}}(\vec{p})$ |
| var. princ. | | $\delta \mathcal{S} = 0\,, \quad \mathcal{S} = \int_{t_1}^{t_2} dt\, \mathcal{L}(\vec{x}, \dot{\vec{x}})$ | $= \int_{t_1}^{t_2} dt\, [\dot{\vec{x}} \cdot \vec{p} - \mathcal{H}(\vec{x}, \vec{p})]$ |
| dynamics | $m\ddot{\vec{x}} = -\mathrm{grad} V(\vec{x})$ | $\frac{\partial \mathcal{L}}{\partial x^i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}^i} = 0$ | $\dot{x}^i = \frac{\partial \mathcal{H}}{\partial p^i}\,, \quad \dot{p}^i = -\frac{\partial \mathcal{H}}{\partial x^i}$ |
| conserved | $E = T + V$ | $\dot{x}^i \frac{\partial \mathcal{L}}{\partial \dot{x}^i} - \mathcal{L} = E$ | $\mathcal{H}(\vec{x}, \vec{p}) = E$ |

**Remark:** The ***observables*** (or physical quantities) are, in genral, functions

$$f \;:\; \mathbb{R}^+ \times E(3) \times E_p(3) \to \mathbb{R}\,, \tag{2}$$

whose values are $f(t, \vec{x}, \vec{p})$.

In the canonical approach (Hamilton) the time evolution of the physical observables is given by the general dynamical equation

$$\frac{df(t,\vec{x},\vec{p})}{dt} = \frac{\partial f(t,\vec{x},\vec{p})}{\partial t} + \{f(t,\vec{x},\vec{p}), \mathcal{H}(\vec{x},\vec{p})\} \tag{3}$$

where the Poisson brackets are defined as

$$\{f,g\} = \sum_i \left( \frac{\partial f}{\partial x^i}\frac{\partial g}{\partial p^i} - \frac{\partial g}{\partial x^i}\frac{\partial f}{\partial p^i} \right) . \tag{4}$$

**Remark** The conserved observables (or prime integrals) are functions $f(\vec{x},\vec{p})$, independent on $t$, which satisfy $\{f,\mathcal{H}\} = 0$.

**Theorem** Given any prime integrals $f$ and $g$ then $\{f,g\}$ is a prime integral.

**Definition** A vector space equipped with an operation $\{\, ,\, \}$ with the properties have the following properties:

$$\{f,g\} = -\{g,f\} \ , \tag{5}$$

$$\{f,\{g,h\}\} + \{g,\{h,f\}\} + \{h,\{f,g\}\} = 0 \, , \tag{6}$$

forms a ***Lie algebra***.

**Conclusion** The set of the conserved observables (or prime integrals) can be organized as a Lie algebra with respect to the Poisson bracket. Moreover, there are other subsets of functions having this property.

**Example 1.** The coordinates and momentum accomplish

$$\left\{x^i, p^j\right\} = \delta_{ij}\,, \quad \left\{x^i, x^j\right\} = 0\,, \quad \left\{p^i, p^j\right\} = 0\,. \tag{7}$$

**Example 2.** The components of the angular momentum $\vec{L} = \vec{x} \wedge \vec{p}$ satisfy

$$\{L_1, L_2\} = L_3\,, \quad \{L_2, L_3\} = L_1\,, \quad \{L_3, L_1\} = L_2\,. \tag{8}$$

**Example 3.** The Laplace-Runge-Lenz vector $\vec{R} = \vec{p} \wedge \vec{L} - \phi(r)\vec{e}_r$, where $\vec{e}_r = \vec{x}/r$ and $r = |\vec{x}|$, was recovered by Pauli and gives rise to the nice algebra

$$\{L_1, R_2\} = R_3\,, \quad \{L_2, R_3\} = R_1\,, \quad \{L_3, R_1\} = R_2\,, \tag{9}$$

$$\{R_1, R_2\} = \chi L_3\,, \quad \{R_2, R_3\} = \chi L_1\,, \quad \{R_3, R_1\} = \chi L_2\,. \tag{10}$$

where

$$\chi = -\vec{p}^{\,2} + \frac{2\phi(r)}{r} + \frac{d\phi(r)}{dr}\,. \tag{11}$$

# Non-relativistic quantum systems

## Experimental evidences

1. The states of the quantum system are determined by a macroscopic apparatus which stops its causal evolution during the experiment. One says that the apparatus ***prepares*** the quantum states.

2. The influence of this apparatus upon the measured quantum systems is out of our hands and, therefore, this remains partially unknown. For this reason there are quantum states with a natural ***statistical*** behavior.

3. In a quantum state some observables can not be measured with the desired accuracy while other ones take ***discrete*** (quantized) values.

4. The quantum systems move (evolve) causally only out of the experiment. Between two measured states the system makes a ***transition***.

## Principles

I. The ***ket*** vectors, $|\ \rangle$, of the space $\mathfrak{K}$, and the associated ***bra*** vectors $\langle\ |$, of the space $\mathfrak{B}$, give rise to the hermitian forms $\langle\ |\ \rangle$. The quantum states are represented by the ket vectors $|\psi\rangle$ of ***finite norm*** ($\langle\psi|\psi\rangle < \infty$) forming the Hilbert space $\mathfrak{H} \subset \mathfrak{K}$.

II. The quantum observables, denoted by $A$, $B$,..., are time-independent ***hermitian*** operators on the space $\mathfrak{K}$, i. e. $A = A^\dagger$ or $\langle\psi|A|\chi\rangle = \langle\chi|A|\psi\rangle^*$ .

III. When one measures the observable $A$ one can obtain only values from its ***spectrum*** $S(A)$. The expectation value of $A$ in the state $|\psi\rangle$ is $\langle\psi|A|\psi\rangle$.

IV. The causal motion of any quantum system is governed by the Schrödinger equation

$$i\hbar\partial_t|\Psi(t)\rangle = H(t)|\Psi(t)\rangle \tag{12}$$

where the ***Hamiltonian*** operator $H(t)$ can depend on time.

## Correspondence

One takes over the classical dynamic associating to each physical quantity a Hermitian operator,

$$x^i \to X^i\,, \quad p^i \to P^i\,, \quad f(\vec{x},\vec{p}) \to f(\vec{X},\vec{P})\,. \tag{13}$$

The next step is to postulate that each Lie algebra of classical quantities is ***represented*** by a Lie algebra of operators whose skew-symmetric operation is just the ***commutator***, $[A,B]=AB-BA$. This enables one to assume

$$\begin{array}{ll} \{x^i,x^j\}=0 & \to [X^i,X^j]=0 \\ \{p^i,p^j\}=0 & \to [P^i,P^j]=0 \\ \{x^i,p^j\}=\delta_{ij} & \to [X^i,P^j]=i\hbar\delta_{ij}I\,. \end{array} \tag{14}$$

where $I$ is the identity operator on $\mathfrak{K}$.

**Definition** The algebra of quantum observables of the spinless systems is freely generated by the operators $X^i$ and $P^i$ giving rise to ***orbital*** operators.

## Representations

**Definition** Each set of ket vectors which forms a ***bases*** in the space $\mathfrak{K}$ determines its own ***representation*** of the QM.
**Remark** The basis vectors can be defined as common eigenvectors of some ***complete sets of commuting operators*** (c.s.c.o.).

**Example 1.** The energy basis $\{|n\rangle\}_{n=0,1,2...}$ of the one-dimensional harmonic oscillator is formed by the eigenvectors obeying $H|n\rangle = E_n|n\rangle$ and $\langle n|m\rangle = \delta_{n,m}$.

**Example 2.** The ***coordinate representation*** is given by the basis $\{|\vec{x}\rangle\}$ of the common eigenvectors of the set $\{X^1, X^2, X^3\}$. These satisfy the eigenvalues equations $X^i|\vec{x}\rangle = x^i|\vec{x}\rangle$ and $\langle\vec{x}|\vec{y}\rangle = \delta^3(\vec{x}-\vec{y})$. Any state $|\psi\rangle \in \mathfrak{H}$ is represented now by the ***static*** wave-function $\psi(\vec{x}) = \langle\vec{x}|\psi\rangle$ while the scalar product has to be written as,

$$\langle\psi|\phi\rangle = \int d^3x \langle\psi|\vec{x}\rangle\langle\vec{x}|\phi\rangle = \int d^3x \psi(\vec{x})^* \phi(\vec{x})\,. \tag{15}$$

**Theorem** In this representation the momentum operators act as the ***differential*** operators $\hat{P}^i$ defined as

$$\langle \vec{x}|P^i|\psi\rangle = (\hat{P}^i\psi)(\vec{x}) = -i\hbar\frac{\partial\psi(\vec{x})}{\partial x_i} \,. \tag{16}$$

Consequently, the Schrödinger equation can be written as a differential equation governed by the Hamiltonian operator $\hat{H}(t)$.

Assuming that there exists another discrete basis $\{|a, b, ...\rangle\}$ of common eigenvectors of the c.s.c.o. $\{A, B, ...\}$,

$$A|a, b, ...\rangle = a|a, b, ...\rangle \,, \quad B|a, b, ...\rangle = b|a, b, ...\rangle \,, ...\text{etc.} \,, \tag{17}$$

with the properties $\langle a, b, ...|a', b', ...\rangle = \delta(a, a')\delta(b, b')...$, we obtain the expansion

$$\psi(\vec{x}) = \langle \vec{x}|\psi\rangle = \sum_{a,b,...} C_{a,b,...}\langle \vec{x}|a, b, ...\rangle \,, \quad C_{a,b,...} = \langle a, b, ...|\psi\rangle \,. \tag{18}$$

## Time evolution

The causal evolution is given by the Schrödinger equation (12). This has a well-determined solution if one know the ***initial*** state $|\Psi(t_0)\rangle = |\psi\rangle$ prepared at time $t_0$.

**Definition** The ***evolution*** operator $U(t,t')$ is unitary, has the algebraic properties $U(t,t) = I$ and $U(t,t')U(t',t'') = U(t,t'')$ and satisfies the equation

$$i\hbar\partial_t U(t,t') = H(t)U(t,t')\,. \tag{19}$$

With this operator we can separate the time evolution from the preparation of the initial state as $|\Psi(t)\rangle = U(t,t_0)|\psi\rangle$.

Turning back to the coordinate representation we find that the wave-function which describes the ***causal*** time evolution can be expanded in the basis $\{|a,b,...\rangle\}$ as

$$\Psi(t,\vec{x}) = \langle\vec{x}|\Psi(t)\rangle = \sum_{a,b,...} C_{a,b,...}\langle\vec{x}|U(t,t_0)|a,b,...\rangle\,, \tag{20}$$

## Quantum modes

Equation (20) can be put in the form

$$\Psi(t,\vec{x}) = \sum_{a,b,...} C_{a,b,...} u_{a,b,...}(t,\vec{x}) \tag{21}$$

where the wave-functions $u_{a,b,...}(t,\vec{x}) = \langle \vec{x}|U(t,t_0)|a,b,...\rangle$ are called often the ***quantum modes*** determined by the c.s.c.o. $\{A, B, ...\}$.

**Remark** Whether all the operators of the c.s.c.o. $\{A, B, ...\}$ ***commute*** with $H(t)$ and implicitly with $U(t,t')$ then the quantum modes are common eigenfunctions of the differential operators $\{\hat{A}, \hat{B}, ...\}$ which act as

$$[\hat{A}u_{a,b,...}(t)](\vec{x}) = \langle \vec{x}|AU(t,t_0)|a,b,...\rangle \tag{22}$$

$$= \langle \vec{x}|U(t,t_0)A|a,b,...\rangle = a u_{a,b,...}(t,\vec{x})\,. \tag{23}$$

The conclusion is that in this case the quantum modes are ***solutions*** of the Schrödinger equation and simultaneously common ***eigenfunctions*** of the c.s.c.o. of differential operators $\{\hat{A}, \hat{B}, ...\}$.

# Relativistic quantum modes

**Looking for relativistic quantum modes**

1. We focus on the relativistic ***free fields*** since these satisfy homogeneous differential equations which transform ***covariantly*** under isometry transformations.

2. We must identify complete sets of commuting differential operators, which commute with the operator of the field equation, being thus able to determine the quantum modes as systems of common eigenfunctions.

3. We need to introduce a relativistic scalar product exploiting an ***internal*** symmetry. This will help us to normalize the quantum modes.

**Remark** The only operators which play the role of conserved quantities are the ***generators*** either of the ***isometries*** of the background or of several ***internal*** symmetries. These operator can be derived in ***Lagrangian*** theories using the ***Noether*** theorem.

## Covariant fields in special and general relativity

Let $(M, g)$ be a physical 4-dimensional Riemannian manifold of metric tensor $g$ whose flat model is just the Minkowski space-time $(M_0, \eta)$ with the metric $\eta = \mathrm{diag}(1, -1, -1, -1)$. In special relativity we have $M = M_0$ and $g = \eta$.

**Definition** The group $G(\eta) = SO(1, 3)$ which preserves the metric $\eta$ is called the ***gauge*** group of $(M, g)$.

The manifold $(M, g)$ may have isometries which transform the local coordinates without to affect the form of the metric tensor. The isometries,

$$x^\mu \to x'^\mu = \phi^\mu_\xi(x) = x^\mu + K^\mu_a(x)\xi^a + ... , \tag{24}$$

form the Lie group $I(M)$ depending on the real parameters $\xi^a$, $a = 1, 2...N$, where $N \leq 10$. The Killing vectors $K_a$ associated to these isometries satisfy the Killing equation $K_{a\,\mu;\nu} + K_{a\,\nu;\mu} = 0$. (The notation $f_{;\mu} = \nabla_\mu f$ stands for the covariant derivatives).

**Definition** The field $\psi : M \to V$ is called ***covariant*** if it transforms under isometries as

$$\psi(x) \to \psi'(x') = Q(x,\xi)\psi(x) = \psi(x') - (i\xi^a X_a \psi)(x') + \dots . \tag{25}$$

where $Q$ are the matrices of a finite-dimensional representation of the gauge group $G(\eta) = SO(1,3)$ carried by the vector space $V$.

**Theorem** The representations $Q : I(M) \to \mathrm{Aut}(V)$ are ***induced*** by the gauge group $G(\eta)$ such that the generators of the transformations (25) are given by Carter and McLenaghan formula

$$X_a = -iK_a^\mu \nabla_\mu + \frac{1}{2} K_{a\,\mu;\nu}\, S^{\mu\nu}\,, \tag{26}$$

where the $S^{\mu\nu}$ are point-wise matrices generating the finite-dimensional representations $D$ of the gauge group.

**Remark** In the Minkowski case the gauge group $SO(1,3)$ is a ***subgroup*** of the isometry one which is the Poincare group $I(M_0) = T(4) \circledS SO(1,3)$. For this reason the fields on $(M_0, \eta)$ transform ***manifestly*** covariant.

## The Lagrangian formalism

The free fields satisfy field equations which can be derived from actions

$$\mathcal{S}[\psi,\bar{\psi}]=\int_{\Delta} d^4x\,\sqrt{g}\,\mathcal{L}(\psi,\psi_{;\mu},\bar{\psi},\bar{\psi}_{;\mu})\,,\quad g=|\det g_{\mu\nu}|\,,\tag{27}$$

depending on the field $\psi$ and its Dirac adjoint $\bar{\psi}$ whose components play the role of canonical variables in the Lagrangian density $\mathcal{L}$.

**Theorem** The action $\mathcal{S}$ is extremal if the fields $\psi$ and $\bar{\psi}$ satisfy the Euler-Lagrange equations

$$\frac{\partial\mathcal{L}}{\partial\bar{\psi}}-\frac{1}{\sqrt{g}}\,\partial_\mu\,\frac{\partial(\sqrt{g}\,\mathcal{L})}{\partial\bar{\psi}_{,\mu}}=0\,,\qquad \frac{\partial\mathcal{L}}{\partial\psi}-\frac{1}{\sqrt{g}}\,\partial_\mu\,\frac{\partial(\sqrt{g}\,\mathcal{L})}{\partial\psi_{,\mu}}=0\,.\tag{28}$$

**Example** If $\psi$ is the scalar field of mass $m$ then $\bar{\psi}=\psi^*$ and the Lagrangian density takes the form $\mathcal{L}=g^{\mu\nu}\partial_\mu\psi^*\partial_\nu\psi-m^2\psi^*\psi$ giving the Klein-Gordon equation

$$\frac{1}{\sqrt{g}}\,\partial_\mu(\sqrt{g}\,g^{\mu\nu}\partial_\nu\psi)+m^2\psi=0\,.\tag{29}$$

**Definition** Any transformation $\psi \to \psi' = \psi + \delta\psi$ leaving the action invariant, $\mathcal{S}[\psi', \bar{\psi}'] = \mathcal{S}[\psi, \bar{\psi}]$, is a symmetry transformation.

**Theorem** ***Noether*** Each symmetry transformation $\psi \to \psi' = \psi + \delta\psi$ gives rise to the current

$$\Theta^\mu \propto \delta\bar{\psi}\frac{\partial\mathcal{L}}{\partial\bar{\psi}_{,\mu}} + \frac{\partial\mathcal{L}}{\partial\psi_{,\mu}}\delta\psi \tag{30}$$

which is conserved in the sense that $\Theta^\mu{}_{;\mu} = 0$.

**Remark** As mentioned before, there are two types of symmetries:

1. ***External*** symmetries (isometries) transforming simultaneously the coordinates and the field components according to equations (24) and (25). In this case $\delta\psi = -i\xi^a X_a \psi$ where $X_a$ are defined by equation (26).

2. ***Internal*** symmetries when only the field components transform as $\psi \to \psi' = D(\zeta)\psi = \psi - i\zeta_A Z^A \psi + ...$ according to the representation $D$ (generated by the matrices $Z^A$) of a unitary group of internal symmetry having the parameters $\zeta^A$ ($A = 1, 2 ... N_{int}$). Now $\delta\psi = -i\zeta_A Z^A \psi$.

## Conserved quantities and the relativistic scalar product

According to the Noether theorem each isometry of parameter $\xi^a$ and each internal symmetry parametrized by $\zeta^A$ produce the corresponding conserved currents

$$\Theta_a^\mu = i\left(\bar{X_a\psi}\,\frac{\partial\mathcal{L}}{\partial\bar{\psi}_{,\mu}} - \frac{\partial\mathcal{L}}{\partial\psi_{,\mu}}\,X_a\psi\right)\,, \quad a = 1,2...N \tag{31}$$

$$\Theta_A^\mu = i\left(\bar{Z_A\psi}\,\frac{\partial\mathcal{L}}{\partial\bar{\psi}_{,\mu}} - \frac{\partial\mathcal{L}}{\partial\psi_{,\mu}}\,Z_A\psi\right)\,, \quad A = 1,2...N_{int}\,. \tag{32}$$

**Theorem** For each conserved current $\Theta^\mu$ there exist a corresponding conserved quantity

$$C = \int_{\partial\Delta} d\sigma_\mu\sqrt{g}\,\Theta^\mu\,, \tag{33}$$

called often conserved charge.

**Definition** The relativistic scalar product $\langle\ ,\ \rangle$ is defined as

$$\langle\psi,\psi'\rangle = i\int_{\partial\Delta} d\sigma_\mu\sqrt{g}\,\left(\bar{\psi}\,\frac{\partial\mathcal{L}'}{\partial\bar{\psi}'_{,\mu}} - \frac{\partial\mathcal{L}}{\partial\psi_{,\mu}}\,\psi'\right)\,. \tag{34}$$

**Corollary** The conserved charged can be represented as expectation values of the symmetry generators using of the relativistic scalar product,

$$C_a = \int_{\partial\Delta} d\sigma_\mu\sqrt{g}\,\Theta^\mu_a = \langle\psi, X_a\psi\rangle\,, \tag{35}$$

$$C_A = \int_{\partial\Delta} d\sigma_\mu\sqrt{g}\,\Theta^\mu_A = \langle\psi, Z_A\psi\rangle\,, \tag{36}$$

**Remark 1.** The operators $X_a$ and $Z_A$ are self-adjoint with respect to this scalar product, i. e. $\langle X\psi,\psi'\rangle = \langle\psi, X\psi'\rangle$.

**Remark 2.** The 'squared norm' $\langle\psi,\psi\rangle$ represents the conserved ***electric*** charge since the generator of the gauge group $U(1)_{em}$ is the identity operator $I$.

# Concluding remarks

**Remark 1.** The relativistic covariant fields are classical fields but which can be interpreted in the quantum manner as forming spaces of wave-functions equipped with invariant scalar products. The quantum observables are the isometry generators $X_a$ which are differential operators.

**Remark 2.** For deriving quantum modes one must start with a c.s.c.o. $\{E, X_1, X_2, ...\}$ including the operator of the field equation, $E$. The quantum modes are the common eigenfunctions of these operators. Finally, these modes must be correctly normalized with respect to the relativistic scalar product. Otherwise, the physical meaning could be dramatically affected.

**Remark 3.** These modes are ***globally*** defined so that the vacuum state is well-defined and stable eliminating thus the kinetic welling effects (e. g. the Unruh and Hawking-Gibbons ones).

**Query:** What happens when there are no isometries ? ***I don't know !***