Chapter 2
Delocalization, Gauge Invariance and Non-regular Representations

1 Delocalization and Gauge Invariance

As discussed in the previous chapter, the physical criterium of regularity of the unitary representations of the Heisenberg group corresponds to the interpretation of the generators q, p as (unbounded) observable variables, so that they must be described by self-adjoint operators. This implies that the states of the system can be described in terms of L^2 wave functions on the spectrum of the position q (or, equivalently, of the momentum p). This amounts to assume that the states of the system have good *localization* properties. The aim of this section is to provide evidence that this innocent looking assumption cannot be adopted for the quantum description of some interesting physical systems.

The physical reason for the lack of regularity is that some generators of the Heisenberg group may not correspond to observables and therefore they need not be described by self-adjoint operators.

A typical example is when the configurations of the quantum systems cannot have L^2 localization. For example, for a quantum particle (typically an electron) in a periodic potential (*Bloch electron*), by Bloch theorem the energy eigenstates, in particular the ground state, are described by quasi periodic wave function, which cannot belong to L^2.

This means that in the representations defined by the Bloch states the "position" variable q does not exist as a (densely defined) self-adjoint operator and therefore the corresponding representation of the Heisenberg group is not regular.

Another class of examples arises if one ask for a quantization of a system with a ground state characterized by the property of being the eigenstate of a canonical observable with continuous spectrum. Then, the unitary one-parameter group generated by the conjugated canonical variable cannot be weakly continuous

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and one has to consider non-regular representations (physically interesting models shall be discussed below).[1]

Quite generally, in order to describe the set of physically relevant states of some physical systems, it is convenient to introduce a canonical algebra $\mathcal{A}_W$ larger than the observable algebra $\mathcal{A}$. Correspondingly, the Heisenberg group G_H generated by the larger algebra $\mathcal{A}_W$ contains as a proper subgroup the group G_{obs}, called the *Heisenberg observable subgroup*. generated by $\mathcal{A}$.

Such a structure is particularly interesting if G_{obs} has a non-trivial center $\mathcal{Z}$. The physical origin and interpretation of such a structure is that the center $\mathcal{Z}$ of G_{obs} defines *gauge transformations*, and the generators of $\mathcal{Z}$ have the meaning of *superselected charges*, since they commute with the observable algebra.

The physical consequence is that the observable algebra has inequivalent representations labeled by the spectrum of $\mathcal{Z}$, called superselected sectors and the variables conjugated to the elements of $\mathcal{Z}$ describe *charge raising/lowering* operators.

The physically motivated condition that one is interested in gauge invariant states implies that they must be invariant under $\mathcal{Z}$, i.e. be eigenstates of the generators of $\mathcal{Z}$. Hence, in such representations the one-parameter groups generated by the variables conjugated to $\mathcal{Z}$ cannot be weakly continuous.

A very simple example is the *two body problem*, if one declares that one does not observe the position of the center of mass. Then, the Heisenberg group generated by the canonical variables q_1, q_2, p_1, p_2 contains as observable subgroup, G_{obs}, the group generated by

$$q = q_1 - q_2, \quad p = (m_2 p_1 - m_1 p_2)/(m_1 + m_2), \quad P = p_1 + p_2.$$

The gauge invariant states are the eigenstates of P; in particular, the ground state of the Hamiltonian

$$H = P^2/2M + p^2/2\mu + V(q_1 - q_2), \quad M \equiv m_1 + m_2, \quad \mu \equiv m_1\, m_2/M,$$

corresponds to the zero eigenvalue of P. Then, the GNS representation of the (twelve dimensional) Heisenberg group defined by such ground state is not regular.

As discussed in the Introduction, the cheap widespread solution of admitting non-normalizable states is mathematically unacceptable, since a non-normalizable cyclic ground state implies that *all* transition amplitudes are divergent.

Actually, for the gauge invariant quantization of gauge models, as the examples mentioned above, rather than considering the fake escape of non-normalizable state

[1]For a mathematical analysis of non-regular representations of the Weyl algebra see the pioneering paper by R. Baume, J. Manuceau, A. Pellet and M. Sirugue, Comm. Math Phys. **38**, 29 (1974); a systematic analysis from the point of view of gauge quantum models is given by F. Acerbi, G. Morchio and F. Strocchi, Jour, Math. Phys. **34**, 899 (1992); Lett. Math. Phys. **27**, 1 (1993); Lett. Math. Phys. **26**, 13 (1992).

vectors, one should better consider non-regular representations of the Heisenberg group, or equivalently of the Weyl algebra. This leads to quantizations in which only the exponentials of some canonical variables (hereafter called singular variables, typically those which are not gauge invariant) can be represented, but not the variables of which they are the formal exponentials.

Rather than working with mathematically inconsistent non-normalizable state vectors one should use non-regular representations built on normalizable cyclic vectors, which yield well defined expectations for the regular canonical variables (typically gauge invariant variables) and (only) for the exponentials of the non-regular ones.

The general lesson from the examples mentioned above is that the standard canonical quantization in terms of the Heisenberg canonical variables q, p, may not always be possible, since the canonical variables do not always have a direct physical interpretation and their spectrum may not be observable. A safer and more general quantization is that done in terms of the Weyl operators, whose existence is related to the much milder requirement of existence of translations and boosts.

2 The Representation Defined by a Translationally Invariant State

We consider for simplicity the one-dimensional case. The group of space translations α_β, $\beta \in \mathbf{R}$, is described by the one-parameter group $V(\beta)$, and a state ω_0 on $\mathcal{A}_W$ is translationally invariant if

$$\omega_0(\alpha_\beta(A)) = \omega_0(V(\beta) A V(\beta)^*) = \omega_0(A), \quad \forall A \in \mathcal{A}_W. \tag{2.2.1}$$

An interesting problem is to characterize the GNS representation π_0 defined by ω_0. As we shall see below, such a representation occurs in the quantization of several physical systems and it is also of interest for analogies between quantum mechanical and gauge field theory models. It is also the prototype of non- regular representations of the Heisenberg group.

Proposition 2.1 *The GNS representation π_0 defined by a pure translationally invariant state ω_0 is unitarily equivalent to the following representation*

$$\omega_0(U(\alpha)\, V(\beta)) = 0, \quad \textit{if} \;\; \alpha \neq 0, \quad \omega_0(V(\beta)) = e^{i\beta\bar{p}}, \;\; \bar{p} \in \mathbf{R}. \tag{2.2.2}$$

Thus, the one-parameter group $U(\alpha)$ is non-regularly represented. The GNS representation space $\mathcal{H}_0$ contains as representative of ω_0 a cyclic vector Ψ_0 such that (denoting by the same symbols the elements of the Weyl algebra and their representatives)

$$V(\beta)\Psi_0 = e^{i\beta\bar{p}}\, \Psi_0, \quad (U(\alpha)\, \Psi_0,\, U(\alpha')\, \Psi_0) = 0, \;\; \textit{if} \;\, \alpha \neq \alpha'. \tag{2.2.3}$$

The linear span D of the vectors $U(\alpha)\Psi_0$, $\alpha \in \mathbf{R}$ is dense in $\mathcal{H}_0$, which is **non-separable**.

The generator of the one-parameter group $U(\alpha)$ does not exist, but nevertheless a generic vector of D

$$\Psi_A = A\Psi_0, \quad A = \sum_{n\in\mathbf{Z}} a_n U(\alpha_n), \quad \{a_n\} \in l^2,$$

may be represented by a wave function $\psi_A(x) = \sum_{n\in\mathbf{Z}} a_n\, e^{i\alpha_n x}$, with scalar product given by the ergodic mean

$$(\psi_A, \psi_A) = \sum_{n\in\mathbf{Z}} |a_n|^2 = \lim_{L\to\infty} (2L)^{-1} \int_{-L}^{L} dx\, \bar{\psi}_A(x)\, \psi_A(x). \tag{2.2.4}$$

The spectrum of $V(\beta)$ is a pure point spectrum.

Proof Quite generally, by Eq. (2.2.1) and the Weyl commutation relations one has, $\forall \beta \in \mathbf{R}$,

$$\omega_0(U(\alpha)\, V(\gamma))) = \omega_0(V(\beta)U(\alpha)\, V(\gamma)V(\beta)^*) = \omega_0(U(\alpha)\, V(\gamma))e^{i\alpha\beta}. \tag{2.2.5}$$

Thus one has

$$\omega_0(U(\alpha)V(\gamma)) = 0, \;\text{ unless }\; \alpha = 0, \quad \omega_0(V(\gamma)) \neq 0. \tag{2.2.6}$$

Hence, the representative of the unitary group $U(\alpha)$, $\alpha \in \mathbf{R}$, is not weakly continuous and the representation is not regular.

In order to completely characterize the representation, we note that the translational invariance of ω_0 implies that the operator $T(\beta)$ defined by

$$T(\beta)\, A\, \Psi_0 = \alpha_\beta(A)\, \Psi_0, \quad T(\beta)\, \Psi_0 = \Psi_0, \quad \forall A \in \mathcal{A}_W,$$

is a unitary operator and satisfies $T(\beta)AT(\beta)^* = \alpha_\beta(A)$. In fact, the mapping $T(\beta)$ (together with its inverse) defined on the dense set $\mathcal{A}_W\Psi_0$ by

$$T(\beta)\Psi_0 = \Psi_0, \quad T(\beta)\, A\, \Psi_0 = \alpha_\beta(A)\Psi_0, \quad \forall A \in \mathcal{A}_W,$$

preserves the scalar product as a consequence of the invariance of ω_0,

$$(T(\beta)A\, \Psi_0, T(\beta)\, B\Psi_0) = (\Psi_0, \alpha_\beta(A^*\, B)\, \Psi_0) = \omega_0(\alpha_\beta(A^* B)) =$$
$$= \omega_0(A^* B) = (A\Psi_0,\, B\Psi_0).$$

Hence, $T(\beta)$ is unitary. Furthermore, by construction $T(\beta)^*\, V(\beta)$ commutes with $\mathcal{A}_W$ (since both $T(\beta)$ and $V(\beta)$ generate the same automorphism), and by the

irreducibility of the representation (following from ω_0 being pure) $T(\beta)^* V(\beta) = e^{i\theta(\beta)}\mathbf{1}$. The group law requires $\theta(\beta) = \bar{p}\beta, \bar{p} \in \mathbf{R}$, and therefore $V(\beta)\Psi_0 = e^{i\bar{p}\beta}\,\Psi_0$. Then, Eq. (2.2.6) implies Eqs. (2.2.2), (2.2.3).
The Weyl operators are represented in the following way:

$$(U(\alpha)\psi)(x) = e^{i\alpha x}\,\psi(x), \quad (V(\beta)\psi)(x) = \psi(x+\beta).$$

The rest of the Proposition follows from a direct check that the cyclic vector defined by the wave function $\psi_{\mathbf{1}} = 1$ yields the same expectations as ω_0; therefore the corresponding GNS representations are unitarily equivalent. Moreover, one has

$$V(\beta)\,U(\alpha)\Psi_0 = e^{i(\bar{p}+\alpha)\beta}\,U(\alpha)\,\Psi_0.$$

3 Bloch Electron and Non-regular Quantization

It is a very good approximation to describe an electron in a periodic crystal by a Schrödinger equation with a periodic potential; for simplicity we consider the one-dimensional case.[2] In this case the Hamiltonian is $H = -d^2/dx^2 + W(x)$, with the potential satisfying the periodicity condition $W(x+a) = W(x)$, for a suitable a.

The spectrum of H is purely continuous, so that the improper eigenvectors, and in particular the improper ground state, are not described by square integrable functions and therefore are not normalizable. On the other hand, much of the wisdom on periodic structures in solids makes extensive use of such improper states and in order to bypass the difficulties of non-normalizability it has becomes standard to restrict the wave functions to an elementary unit cell. At the basis of this prescription is the so called Floquet-Bloch theorem,[3] according to which the energy improper eigen-functions can be chosen of the form

$$\psi_k^n(x) = e^{ikx} v_k^n(x), \quad v_k^n(x+a) = v_k^n(x), \quad k \in [0, 2\pi/a), \quad n \in \mathbf{N}, \qquad (2.3.1)$$

(*Bloch electrons*). Such improper states do not play the mere role of limiting extrapolations of well defined vectors (like the plane waves in the free case), since all the physically relevant states used in the treatment of periodic structures in solids belong to the cyclic representation defined by the ground state and the

[2]For an excellent treatment of the Schrödinger operators with periodic potentials, see M. Reed and B. Simon, *Methods of Modern Mathematical Physics, Vol. IV*, Academic Press 1978, Sect. XIII.16; in particular pp. 287–301 for the one-dimensional case. For an expository presentation of the one-dimensional case, see e.g. A.A. Cottey, Am. J. Phys. **39**, 1235 (1971). For the discussion of the related physical problem see e.g. J.M. Ziman, *Principles of the Theory of Solids*, Cambridge Univ. Press 1964, Chap. 1; N.W. Ashcroft, *Solid State Physics*, Saunders College Publ. 1976, p. 132–141.

[3]G. Floquet, Ann. École Norm. Sup. **12**, 47 (1883); W. Magnus and S. Winkler, *Hill's Equation*, Wiley 1966; F. Bloch, Z. Physik **52**, 555 (1928).

latter corresponds to the improper wave function $\psi_0^0(x) = v_0^0(x)$ (Eq. (2.3.1) with $k = 0, n = 0$). This justifies to look for a mathematical control of the status of such representations also in order to obtain well defined rules for computing transition amplitudes etc.

Another motivation for such an investigation is to clarify the analogy drawn between the θ vacua representations in quantum chromodynamics (QCD) and that of the ground state of the Bloch electron.[4]

Proposition 3.1 [5] *Let $W(x)$ be a bounded measurable periodic potential, $W(x) = W(x + a)$, then there exists one and only one irreducible representation $(\pi, \mathcal{K})$ of the CCR algebra $\mathcal{A}_W$ in which the Hamiltonian*

$$H = p^2/2 + W(x)$$

is well defined, as a strong limit of elements of $\mathcal{A}_W$ (on a dense domain), and has a ground state $\Psi_0 \in \mathcal{K}$.

Moreover, such a representation is independent of W, in the class mentioned above, and it is the unique non-regular representation π_0 in which the subgroup $V(\beta)$, $\beta \in \mathbf{R}$ is regularly represented; its generator p has a discrete spectrum.

The Hilbert space $\mathcal{K}$ of π_0 consists of the formal sums

$$\psi(x) = \sum_{n \in \mathbf{Z}} c_n\, e^{i\alpha_n x}, \quad \{c_n\} \in l^2(\mathbf{C}), \quad x \in \mathbf{R}, \quad \alpha_n \in \mathbf{R}, \tag{2.3.2}$$

with scalar product given by the ergodic mean

$$(\psi, \psi) = \sum_{n \in \mathbf{Z}} |c_n|^2 = \lim_{L \to \infty} (2L)^{-1} \int_L^L dx\, \bar{\psi}(x)\, \psi(x). \tag{2.3.3}$$

The Weyl operators are represented by

$$(\pi_o(U(\alpha))\psi)(x) = e^{i\alpha x}\psi(x), \quad (\pi_0(V(\beta))\psi)(x) = \psi(x + \beta). \tag{2.3.4}$$

The (orthogonal) decomposition of $\mathcal{K}$ over the spectrum of $V(a)$ is

$$\mathcal{K} = \sum_{\theta \in [0, 2\pi)} \oplus\, \mathcal{H}_\theta, \quad V(a)\, \mathcal{H}_\theta = e^{i\theta}\, \mathcal{H}_\theta, \quad \theta \in [0, 2\pi). \tag{2.3.5}$$

[4]R. Jackiw, Rev. Mod. Phys. **49**, 681 (1977), Sect. III. G.

[5]J. Löffeholz, G. Morchio and F. Strocchi, Lett. Math. Phys. **35**, 251 (1995).

The spectrum of p in $\mathcal{H}_\theta$ is $\sigma(p)|_{\mathcal{H}_\theta} = \{2\pi n/a + \theta/a,\ n \in \mathbf{Z}\}$ and the wave functions $\psi_\theta \in \mathcal{H}_\theta$ are quasi periodic of the form

$$\psi_\theta(x) = e^{i\theta x/a} \sum c_n e^{i2\pi n x/a}. \tag{2.3.6}$$

*(**Bloch waves**). The unique ground state is a vector of $\mathcal{H}_{\theta=0}$.*

Proof

1) *The representation is non-regular for $U(\alpha)$.*
A bounded measurable potential belongs to the strong closure of $\mathcal{A}_W$ and therefore if H is a well defined operator as a strong limit of elements of $\mathcal{A}_W$, so is $H_0 = p^2/2m$. Hence, p^2 is well defined and so is its square root p, which is the generator of $V(\beta)$. Therefore, by Stone's theorem $V(\beta)$ is weakly continuous, i.e. regularly represented in H.
The Weyl commutation relations and the weak continuity of $V(\beta)$ imply $U(\alpha)\, p\, U(-\alpha) = p - \alpha$, i.e. the spectrum $\sigma(p)$ of p is homogeneous. From the irreducibility of π_0 it follows that three cases are possible:

   i) $\sigma(p)$ is absolutely continuous; hence, by irreducibility $\sigma(p)$ has no multiplicity, so that $U(\alpha)$ act as translations on $\sigma(p)$ and the absolute continuity of the spectral measures of p with respect to the Lebesgue measure implies that $U(\alpha)$ is weakly continuous. Then, by the SvN theorem the representation is equivalent to the Schrödinger representation and there is no ground state;
   ii) $\sigma(p)$ is a pure point spectrum; then, if Ω_λ is a state corresponding to an eigenvector of p with eigenvalue λ, one has, $\forall A \in \mathcal{A}_W$, $\Omega_\lambda(A\, V(\beta)) = e^{i\lambda\beta}\, \Omega_\lambda(A)$, and

$$\Omega_\lambda(U(\alpha)V(\beta)) = \Omega_\lambda(V(\gamma)U(\alpha)\, V(\beta)V(-\gamma)) = e^{i\alpha\gamma}\,\Omega_\lambda(U(\alpha)\, V(\beta)),$$

   i.e.

$$\Omega_\lambda(U(\alpha)V(\beta)) = 0, \quad \forall \alpha \neq 0, \quad \Omega_\lambda(V(\beta)) = e^{i\lambda\beta}.$$

   In conclusion, the representation is unitarily equivalent to the *non-regular* representation of a translationally invariant state, Proposition 2.1. Then, Eqs. (2.3.2), (2.3.3) hold;
   iii) $\sigma(p)$ is purely singular, to be discussed later.

2) *The spectrum of $V(a)$ and of the Hamiltonian.*
In such a representation the potential can be written in the following form $W(x) = \sum_n v_n\, U(2\pi n/a)$, where v_n are the coefficients of the Fourier expansion of the periodic function $W(x)$ in $[0, a]$ and the series is strongly convergent on D. For the analysis of the spectrum of H, since $V(a) = e^{ipa}$ commutes with H, it is convenient to decompose $\mathcal{K}$ according to the spectrum of $V(a)$, which is purely discrete and coincides with the whole circle, (Eq. (2.3.5)).

Then,

$$\psi(x) = \sum_n c_n U(\alpha_n)\psi_{\mathbf{1}} = \sum_n c_n \exp(i\alpha_n x) \in \mathcal{H}_\theta,$$

implies $V(a)\psi(x) = e^{i\theta}\,\psi(x)$ and on the other hand, by the Weyl commutation relations,

$$V(a)\sum_n c_n U(\alpha_n)\,\psi_{\mathbf{1}} = \sum_n c_n e^{i\alpha_n(x+a)}.$$

Hence, one must have $\alpha_n = \theta/a + 2\pi n/a$, $n \in \mathbf{Z}$ and $\psi(x)$ can be written as in Eq. (2.3.6), i.e. $\psi(x)$ is a quasi periodic function of the form of Eq. (2.3.1), with $k = \theta/a$.

3) *The unique ground state belongs to* $\mathcal{H}_{\theta=0}$.

Since $V(a)$ commutes with H, the subspaces $\mathcal{H}_\theta$ reduce $\mathcal{K}$ and in $\mathcal{H}_\theta$ the Hamiltonian reduces to $H_\theta = H_{0,\theta} + W(x)$, $H_{0,\theta} = p_\theta^2/2m$. Since $W(x)$ is bounded, it is a bounded operator in each $\mathcal{H}_\theta$ and therefore it is infinitesimally smaller than $H_{0,\theta}$ in the sense of Kato, (i.e. $||W\psi_\theta|| \leq a||H_{0,\theta}\psi_\theta|| + b||\psi_\theta||$, with $\inf a = 0$). Since the spectrum of $H_{0,\theta}$ is discrete, so is the spectrum of H_θ; this implies that ground states exist.

Moreover, the boundedness of $W(x)$ in $\mathcal{H}_\theta$ implies that e^{-H_θ} has a strictly positive kernel, i.e. $e^{-H_\theta}\,\psi_\theta(x) > 0$, $\forall \psi_\theta \geq 0$. Now, if $\Psi_0 \in \mathcal{H}$ is the ground state, it must have a non-vanishing projection $\psi_{0,\theta}$ on at least one $\mathcal{H}_\theta$, corresponding to $\inf\ \sigma(H_\theta)$. By a generalized Perron-Frobenius theorem the corresponding wave function may be chosen strictly positive

$$\mathcal{H}_\theta \ni \psi_{0,\theta}(x) = e^{i\varphi}|\psi_{0,\theta}(x)|,\ \varphi \in \mathbf{R},\ \ |\psi_{0,\theta}(x)| \neq 0,\ \ a.e. \tag{2.3.7}$$

Since $|\psi_{0,\theta}(x)|$ is a periodic function, it belongs to $\mathcal{H}_{\theta=0}$ and Eq. (2.3.7) is consistent only for $\theta = 0$. The ground state is unique because any other ground state would be described by a positive wave function and therefore could not be orthogonal to Ψ_0.[6]

iii) The possibility of a representation characterized by a purely singular $\sigma(p)$ is excluded by the following argument. As in the previous case, one may decompose the Hilbert space $\mathcal{K}$ of such a representation according to the spectrum of $V(a)$, $\mathcal{K} = \int d\nu(\theta)\,\mathcal{K}_\theta$, with a measure $d\nu(\theta)$ now singular with respect to the Lebesgue measure and translationally invariant because

[6]For the permanence of a discrete spectrum under a bounded perturbation see M. Reed and B. Simon, *Methods of Modern Mathematical Physics, Vol. IV*, Academic Press 1972, Theors. XII.11, XII.13. For the generalized Perron-Frobenius theorem see J. Glimm and A. Jaffe, *Quantum Physics. A Functional Integral Point of View*, Springer 1987, Sect. 3.3; for a simple account see F. Strocchi, *An Introduction to the Mathematical Structure of Quantum Mechanics*, 2nd ed., World Scientific 2008, Sect. 6.4.

$\tilde{U}(\alpha) \equiv U(\alpha/a)$ maps $\mathcal{K}_\theta$ into $\mathcal{K}_{\theta+\alpha}$. In each space $\mathcal{K}_\theta$ corresponding to such a decomposition, the spectrum of p is discrete and coincides there with the spectrum in the subspace $\mathcal{H}_\theta$ of the preceding case. Then, the representation of the subalgebra generated by $V(\beta)$, $\beta \in \mathbf{R}$ and by $U(2\pi n/a)$, $n \in \mathbf{Z}$, is quasi equivalent to that in $\mathcal{H}_\theta$. The Hamiltonian H is therefore defined in $\mathcal{K}_\theta$ and has the same spectrum as in $\mathcal{H}_\theta$; by the same arguments if inf $\sigma(H)$ is an eigenvalue the corresponding eigenvector must belong to $\mathcal{K}_{\theta=0}$, which must therefore appear as a discrete component of $\mathcal{K}$. Since the spectrum of p is purely discrete in $\mathcal{K}_{\theta=0}$, by irreducibility it is purely discrete in $\mathcal{K}$ and has no singular component there.

The above theorem allows to recover in a simple (mathematically rigorous) way the basic features of the analysis of the energy spectrum in the case of periodic potentials.[7]

a) **Band structure**. The energy spectrum $\{E_n(\theta)\}$ is characterized by bands, classified by the quantum number $n \in \mathbf{Z}$; within each band the energy levels are functions of the parameter $\theta \in [0, 2\pi/a)$.
b) **Description in terms of the elementary cell**. Equation (2.3.6) defines an isomorphism between $\mathcal{H}_\theta$ and $L^2([0,a), dx/a)$, so that the scalar product in $\mathcal{H}_\theta$ reduces to an L^2 product with integration over the *elementary cell* [0, a]. In this identification, p is represented by the self adjoint extension of the differential operator $-id/dx$, corresponding to the boundary conditions $\psi(a) = e^{i\theta}\,\psi(0)$. The generic function $\psi \in \mathcal{K}$ can be expressed as a denumerable superposition of ψ_{θ_k}

$$\psi(x) = \sum_{\theta_k} c(\theta_k)\psi_{\theta_k}(x)$$

and since $(\psi_\theta, \varphi_{\theta'}) = 0$ if $\theta \neq \theta'$, the product (2.3.3) reduces to a sum of products in $L^2([0,a], dx/a)$, i.e. in the elementary cell.

The energy is a continuous function of θ, since $\tilde{U}(\theta) : \mathcal{H}_{\theta=0} \to \mathcal{H}_\theta$, so that

$$(\psi_\theta, H\,\psi_\theta) = (\psi_0, (H + p\theta/m + \theta^2/2m)\,\psi_0).$$

[7] M. Reed and B. Simon, *Methods of Modern Mathematical Physics, Vol. IV*, Academic Press, Sect. XIII.16.

4 Gauge Invariance and Non-regular Canonical Quantization

4.1 Gauge Invariance and Superselection Rules

A general case leading to non-regular representations is when (i) a quantum system is described by canonical variables, generating a Heisenberg group G_H, but only a subset of them, and consequently only a subgroup $G_{obs} \subset G_H$, describes observable quantities, (ii) G_{obs} is generated by a Heisenberg subgroup and by an abelian subgroup $\mathcal{G}$ which commutes with G_{obs}. Then, $\mathcal{G}$ generates a group of transformations α_g, $g \in \mathcal{G}$, which leave the observables pointwise invariant

$$\alpha_g(A) = A, \quad \forall A \in G_{obs}, \quad \forall g \in \mathcal{G}, \tag{2.4.1}$$

i.e. $\mathcal{G}$ has the meaning of a **gauge group**,.

The elements of G_H generate a C^*-algebra $\mathcal{F}_W$, called *field algebra*, and the elements of G_{obs} generate a *C^*-algebra $\mathcal{A}$ of observables*, characterized by gauge invariance, Eq. (2.4.1) (as discussed in Chap. 1, Sect. 3). $\mathcal{A}$ has a non-trivial *center* $\mathcal{Z}$ generated by the elements of $\mathcal{G}$. A representation of $\mathcal{F}_W$ is *physical* if G_{obs} is regularly represented.

In the irreducible representations of $\mathcal{A}$, $\mathcal{Z}$ is represented by multiples of the identity. The generators of $\mathcal{G}$ have the meaning of **superselected charges** and the points θ of the spectrum $\sigma(\mathcal{Z})$ of $\mathcal{Z}$ label inequivalent representations $(\mathcal{H}_\theta, \pi_\theta)$ of $\mathcal{A}$, called **$\boldsymbol{\theta}$ sectors**. Stone-von Neumann uniqueness theorem does not apply and this can be traced back to the fact that, contrary to the Weyl C^*-algebra, $\mathcal{A}$ is not simple.

By definition a *gauge invariant state ω* on $\mathcal{F}_W$ satisfies $\omega(\alpha_g(F)) = \omega(F)$, $\forall F \in \mathcal{F}_W$ and therefore, in the GNS representation π_ω of $\mathcal{F}_W$ defined by ω, the gauge transformations are implemented by unitary operators $U(g)$ defined by (Ψ_ω denotes the vector which represents ω)

$$U(g)\Psi_\omega = \Psi_\omega, \quad U(g)\pi_\omega(F)\Psi_\omega = \pi_\omega(\alpha_g(F))\,\Psi_\omega, \quad \forall F \in \mathcal{F}_W.$$

Let $V(g)$ denote the element of $\mathcal{G}$ which defines α_g: $\alpha_g(F) = V(g)\,F\,V(g)^{-1}$, $\forall F \in \mathcal{F}_W$; then, $\pi_\omega(V(g))U(g)^*$ commutes with $\mathcal{F}_W$ and, in each irreducible representation of $\mathcal{F}_W$, $\pi_\omega(V(g))\,U(g)^* = e^{i\theta(g)}\mathbf{1}$. Hence, Ψ_ω is an eigenvector of $\pi_\omega(V(g))$, with eigenvalue $e^{i\theta(g)}$,

$$\pi_\omega(V(g))\Psi_\omega = \pi_\omega(V(g))U(g)^*\Psi_\omega = e^{i\theta(g)}\Psi_\omega. \tag{2.4.2}$$

Thus, the analysis of Sect. 2, applies, with the result that the GNS representation π_ω of $\mathcal{F}_W$, equivalently of G_H, defined by a gauge invariant state ω is non-regular,

$$\mathcal{H}_{\pi_\omega} = \sum_{\theta \in \sigma(\mathcal{Z})} \oplus \mathcal{H}_\theta,$$

and the subspaces $\mathcal{H}_\theta$ carrying disjoint irreducible representations of $\mathcal{A}$ are proper subspaces of the non-separable space $\mathcal{H}_{\pi_\omega}$.

Proposition 4.1 *Let G_H be the Heisenberg group defined by the set of canonical variables $\{q_i, p_i\}$, $\mathcal{F}_W$ the corresponding canonical C^*-algebra, $\mathcal{A} \subset \mathcal{F}_W$ the C^*-subalgebra of observables and $\mathcal{G}$ the commutative group of gauge transformations, defined by a subgroup $\mathcal{G} \subset G_H$.*

Then, the GNS representation of $\mathcal{F}_W$ defined by a gauge invariant state is a non-regular representation of $\mathcal{F}_W$, as well as of the Heisenberg group G_H, and the elements of $\mathcal{G}$ define **superselection rules**.

Relevant examples of such a structure are provided by quantum mechanical models, in particular those exhibiting strong analogies with gauge quantum field theories (see in particular the following chapter).

4.2 Gauge Invariance in the Two-Body Problem

The description of the quantum two-body problem is provided by the Weyl field algebra $\mathcal{F}_W$ generated by the exponentials $u(\alpha)$, $v(\beta)$ of the center of mass canonical variables Q, P, and by the exponentials $U(\alpha)$, $V(\beta)$ of the relative canonical variables q, p. The Hamiltonian has the form

$$H = P^2/2M + p^2/2\mu + V(q) \tag{2.4.3}$$

and, for the purpose of discussing the bound state spectrum and in particular the lowest energy level, the position of the center of mass is irrelevant. It is therefore natural to consider as observable C^*-algebra $\mathcal{A}$ the algebra generated by the canonical variable q, p, P. Since the center of mass position is not observed, the translations $v(\beta)$ of the center of mass have the meaning of *gauge transformations*.

Therefore, the representations of the canonical field algebra $\mathcal{F}_W$ defined by a gauge invariant state ω are characterized by the property that the vector Ψ_ω, which represents ω, is an eigenvector of $v(\beta)$, equivalently of P. In particular, the lowest energy state ω_0 must satisfy $\omega_0(P^2) = 0$, so that the corresponding vector Ψ_0 satisfies

$$0 = (\Psi_0, P^2\, \Psi_0) = ||P\, \Psi_0||^2, \quad \text{i.e.} \quad P\, \Psi_0 = 0. \tag{2.4.4}$$

As discussed in Sect. 2, the representations of the canonical algebra $\mathcal{F}_W$ defined by gauge invariant states are non-regular; in fact, Eq. (2.4.4) is incompatible with the canonical commutation relations in the Heisenberg form. It has been suggested to bypass such incompatibility by allowing Ψ_0 to be non-normalizable.[8] In our opinion, such a choice would have catastrophic consequence on the GNS representation defined by such a ground state; by the cyclicity of Ψ_0 all vectors of such a representation would be non-normalizable, all matrix elements (including the ground state expectations of gauge invariant operators) would be divergent and one could not extract finite results in a consistent mathematical way.

However, Eq. (2.4.4) is compatible with the CCR in Weyl form. Thus, a canonical quantization is not forbidden, provided it is done in terms of the Weyl algebra, rather than of the Heisenberg algebra; actually, it is uniquely determined and coincides with the non-regular representation discussed in Sect. 2. The vector states are not represented by square integrable functions on the spectrum of Q, but one can still describe them by wave functions of the center of mass position by using a non-L^2 scalar product (see Eq. (2.2.4)).

In our opinion, from a mathematical point of view, the non-regularity of the representation is a much better price to pay, rather than living with non-normalizable state vectors. The advantages of such a quantization is that the states are described by *normalizable* vectors of a Hilbert space, the basic quantum mechanical rules are not violated, the observable subalgebra $\mathcal{A}$ is regularly represented in the standard way, the canonical variables which are not gauge invariant are non-regularly represented, only their exponentials being well defined.

The quantization discussed above sheds light on the quantization of gauge field theories, in particular on the quantization of the temporal gauge.[9]

4.3 Non-regular Representations and Symmetry Breaking

We briefly recall that, given a C^*-algebra $\mathcal{A}$, an algebraic *symmetry* is an automorphism β of $\mathcal{A}$; given a state ω, the symmetry is *unbroken* in the corresponding representation space if β is implemented by a unitary operator $T(\beta)$ there, i.e.

$$\pi_\omega(\beta(A)) = T(\beta)\,\pi_\omega(A)\,T(\beta)^*, \quad \forall A \in \mathcal{A}. \tag{2.4.5}$$

This means that the representation defined by the state ω_β, $\omega_\beta(A) \equiv \omega(\beta(A))$ is unitary equivalent to π_ω:

$$\pi_{\omega_\beta}(A) = T(\beta)\,\pi_\omega(A)\,T^*(\beta).$$

[8] R. Jackiw, Topological Investigations of Quantized Gauge Theories, in S.B. Treiman, R. Jackiw, B. Zumino and E. Witten, *Current Algebra and Anomalies*, World Scientific 1985.

[9] J. Löffelholz, G. Morchio and F. Strocchi, J. Math. Phys. **44**, 5095 (2003).

In this case, β gives rise to a Wigner symmetry in $\mathcal{H}_\omega$, i.e. all transition amplitudes are invariant. Otherwise, if there is no unitary operator which implements β in $\mathcal{H}_\omega$, by Wigner theorem on symmetries at least one transition amplitude is not invariant and the symmetry β is said to be *broken* in $\mathcal{H}_\omega$. An algebraic symmetry is said to be *regular* if it maps regular representations into regular ones.[10]

In the case of quantum systems described by the canonical Weyl algebra, any regular algebraic symmetry is unbroken in any regular irreducible representation, since, by Stone-von Neumann theorem, all such representations are unitarily equivalent. Thus, the important phenomenon of *symmetry breaking*, in the strong sense of a loss of symmetry as defined above, (not merely as the non-invariance of the ground state) cannot appear in the case of Heisenberg quantization, more generally in the case of regular Weyl quantization.

The situation drastically changes in the case of non-regular Weyl quantization. A distinguished case is when one has the structure discussed in Sect. 4.1, namely a canonical algebra $\mathcal{F}_W$ and an observable (gauge invariant) subalgebra $\mathcal{A}$, with a non-trivial center $\mathcal{Z} \subset \mathcal{A}$.

Clearly, any symmetry β of $\mathcal{A}$, defined by an element of $\mathcal{F}_W$, is implemented by a unitary operator $T(\beta)$ in the non-regular representation π of $\mathcal{F}_W$, defined by a gauge invariant state ω_θ, $\theta \in \sigma(\mathcal{Z})$.

However, if β does not commute with the gauge group $\mathcal{G}$, β is broken in *each* irreducible representation $\mathcal{H}_\theta$ of the observable subalgebra $\mathcal{A}$, i.e. β fails to define a Wigner symmetry of the gauge invariant states of $\mathcal{H}_\theta = \overline{\mathcal{A}\,\Psi_{\omega_\theta}}$, because $T(\beta)$ does not leave $\mathcal{H}_\theta$ invariant.

In the regular irreducible representation, π_r of $\mathcal{F}_W$, the symmetry β is unbroken but the elements of $\mathcal{Z}$ have a continuous spectrum in $\mathcal{H}_{\pi_r}$ and there is no gauge invariant (proper) state vector in $\mathcal{H}_{\pi_r}$.

Proposition 4.2 *Let $\mathcal{F}_W$ denote the canonical field C^*-algebra defined by a Heisenberg group G_H, $\mathcal{A}$ the observable C^*-subalgebra, $\mathcal{Z}$ the non-trivial center of $\mathcal{A}$ generated by the commutative subgroup $\mathcal{G} \subset \mathcal{G}_H$ (gauge group), then*

i) any algebraic symmetry β of $\mathcal{A}$, defined by an element of G_H which does not commute with $\mathcal{G}$, is spontaneously broken in each irreducible representation of $\mathcal{A}$ (θ sector);

ii) in any representation of $\mathcal{F}_W$ defined by a gauge invariant state ω, the one-parameter subgroups which do not commute with $\mathcal{G}$ are non-regularly represented, so that the corresponding generators cannot be defined as operators in $\mathcal{H}_\omega$, only their exponentials exist.

For representations of $\mathcal{A}$ defined by a ground state ω_0, (more generally by a state ω invariant under time translations), the non-invariance of ω_0,

$$< A > \equiv \omega_0(A) \neq \omega_0(\beta(A)), \quad \text{for some} \quad A \in \mathcal{A}, \tag{2.4.6}$$

[10]For a discussion of the meaning and the mechanism of spontaneous symmetry breaking see: F. Strocchi, *Symmetry Breaking*, 2nd ed., Springer 2008.

is still compatible with β giving rise to a Wigner symmetry in the GNS representation space $\mathcal{H}_{\omega_0}$. In this case, if β commutes with the dynamics, Eq. (2.4.6) implies degeneracy of the ground state. This is what happens if (2.4.6) holds for β defined by an element of the field algebra $\mathcal{F}_W$ which commutes also with the gauge group.

A one-parameter group β^λ, $\lambda \in \mathbf{R}$, of symmetries shall be called a *continuous symmetry*. A symmetry is called *internal* if it commutes with the one-parameter group α_t, $t \in \mathbf{R}$, of the time translations. In the following, the breaking of an internal symmetry shall be called *spontaneous symmetry breaking*.

4.4 Goldstone Theorem and Non-regular Representations

The spontaneous breaking of a continuous symmetry in the quantum theory of infinitely extended systems is usually accompanied by a strong constraint on the energy spectrum; in fact, if the symmetry commutes with the dynamics (i.e. if the Hamiltonian is symmetric) the Goldstone theorem predicts the absence of an energy gap with respect to the ground state, in the channels related to the ground state by the broken generators.[11]

Here, we investigate a possible *quantum mechanical version of the Goldstone theorem* which mimics as closely as possible the formulation and proof for infinitely extended quantum systems.

For this purpose, given a C^*-algebra $\mathcal{A}$, a one-parameter group β^λ, $\lambda \in \mathbf{R}$ of automorphisms of $\mathcal{A}$ and a representation π of $\mathcal{A}$ defined by a ground state ω_0, we consider :

i) the infinitesimal variation of a generic element $F = \pi(A)$, $A \in \mathcal{A}$,

$$\delta F = \delta(\pi(A)) = \frac{d\,\pi(\beta^\lambda(A))}{d\lambda}|_{\lambda=0},$$

ii) the generation of the continuous symmetry β^λ by elements of the strong closure $\pi(\mathcal{A})''$ of $\pi(\mathcal{A})$, in the sense that there is a sequence $Q_n = Q_n^* \in \pi(\mathcal{A})''$, $n = 1, ..,$ such that

$$\delta F = i \lim_{n\to\infty} [\, Q_n,\, F\,].$$

If Q_n converges weakly to a self adjoint operator Q, then β^λ is implementable by the unitary operator $e^{i\lambda Q}$, the symmetry is not broken and $< \delta F > \equiv \omega_0(F) \neq 0$ implies that ω_0 is not invariant, i.e. $Q\Psi_0 \neq 0$. Furthermore, if β^λ commutes with the time translations α_t, $\Psi_\lambda \equiv e^{i\lambda Q}\Psi_0$ is a family of *degenerate ground*

[11] For a review and critical discussion of the Goldstone theorem see F. Strocchi, *Symmetry Breaking*, 2nd ed., Springer 2008, Chap. 15.

states. In this case, one gets a picture close to the standard heuristic formulation of spontaneous breaking of a continuous symmetry, based on the following oversimplified assumptions: (i) the continuous symmetry is generated by a charge Q, in the sense that $\delta F = i[Q, F]$, (ii) the Hamiltonian is symmetric, i.e. $[Q, H] = 0$, (iii) $< \delta F > \neq 0$; the conclusion being that $Q\Psi_0 \neq 0$ has zero energy.

Closer to the infinite-dimensional case is the case in which there is no sequence Q_n, with the above property, which converges weakly to a self-adjoint operator Q; then, if $< \delta F > \neq 0$, the symmetry is broken in the strong sense of loss of symmetry and $< \delta F >$ is the strict analog of a *symmetry breaking order parameter*, which characterizes symmetry breaking in quantum field theory or in many body theory. Similarly, $< \delta F >= i \lim_{n\to\infty} < [Q_n, F] >$ plays the role of the *symmetry breaking Ward identity*.

If β^λ commutes with α_t, then, by the invariance of the ground state under α_t, one has

$$\lim_{n\to\infty} < [Q_n(t), F] >= \lim_{n\to\infty} < [\alpha_t(Q_n), F] >=$$

$$\lim_{n\to\infty} < [Q_n, \alpha_{-t}(F)] >= -id < \beta^\lambda(\alpha_{-t}(F)) > /d\lambda|_{\lambda=0} = -id < \beta^\lambda(F) > /d\lambda|_{\lambda=0}$$

$$= \lim_{n\to\infty} < [Q_n, F] > .$$

It is worthwhile to stress that such a time independence of the Ward identity holds also in the more general case in which the symmetry does not commute with the Hamiltonian, $\lim_{n\to\infty}[Q_n(t), H] = A \neq 0$, but $< [A, F] >= 0$ (in analogy with the so-called anomaly occurring in the infinite-dimensional case). This is, e.g., the case in which the Hamiltonian is invariant up to a time derivative which commutes with F (see the example of the Bloch electron discussed below).

Theorem 4.3 *Let β^λ, $\lambda \in \mathbf{R}$, be a one-parameter group of automorphisms of the algebra $\mathcal{A}$, α_t the one-parameter group of time translations and π the representation defined by a ground state ω_0. If for some $F \in \pi(\mathcal{A})$,*

$$< \delta F >\equiv d < \beta^\lambda(F) > /d\lambda|_{\lambda=0} \neq 0,$$

$$< \delta F >= i \lim_{n\to\infty} < [Q_n, F] >= i \lim_{n\to\infty} < [Q_n(t), F] >, \tag{2.4.7}$$

for a suitable sequence of $Q_n = Q_n^*$, $Q_n(t) \equiv \alpha_t(Q_n)$, the limit being understood in the sense of convergence of tempered distributions in the variable t, then there is no energy gap above the ground state. Actually, there is a state (Goldstone-like state) orthogonal to the ground state, with the ground state energy.

Proof It is enough to consider the case in which $F = F^*$, since if $F = F_1 + iF_2$, $F_i = F_i^*$, $i = 1, 2$, by linearity the symmetry breaking condition must hold for at least one F_i. Since the representation is defined by a ground state, $\alpha(t)$ is implemented by a one-parameter group of unitary operators $U(t)$, $t \in \mathbf{R}$, with the generator normalized so that the ground state has zero energy. Without loss of generality one can assume that $< Q_n >= 0$, since Eq. (2.4.7) holds also for $\tilde{Q}_n \equiv Q_n - < Q_n >$. Then, one has

$$2\,\mathrm{Im} \lim_{n\to\infty} < Q_n U(-t) F >= i \lim_{n\to\infty} < [Q_n, F] > \neq 0. \tag{2.4.8}$$

The distributional convergence of $J_n(t) \equiv 2\,\mathrm{Im} < Q_n U(-t) F >$ and Eq. (2.4.7) imply the following distributional convergence of the Fourier transforms $\tilde{J}_n(\omega)$

$$\lim_{n\to\infty} \tilde{J}_n(\omega) =< \delta F > \ \delta(\omega).$$

Then, by using the spectral representation $U(t) = \int e^{-i\omega t}\, dE(\omega)$, one concludes that the energy spectral measure contains a $\delta(\omega)$.
The ground state ω_0 cannot be responsible for such a point spectrum, since its contribution as intermediate state in the right hand side of Eq. (2.4.7) vanishes as a consequence of $< Q_n >= 0$; hence there is a zero energy eigenvector orthogonal to the ground state vector.

Remarks A few remarks may be useful.

The statement that the infinitesimal variations under the symmetry transformations is given by a limit of commutators with charges Q_n does not require that, in the given ground state representation, β^λ is implemented by a weakly continuous group of unitary operators.

In the infinite-dimensional cases of quantum field theory and of many body theory, the generation of the symmetry is through the commutator of local charges, typically the integrals of the charge density $j_0(\mathbf{x}, t)$ of a conserved current $j_\mu(\mathbf{x}, t)$ ($\partial^\mu j_\mu = 0$):

$$\delta F = i \lim_{R\to\infty} [Q_R, F], \quad Q_R = \int_{|\mathbf{x}|\leq R} dx\, j_0(\mathbf{x}, t)$$

and $< \delta F > \neq 0$ implies that the commutator $[Q_R, F]$ does not converge to the commutator of a charge Q; therefore Q_R is not weakly convergent to a well defined global charge Q. Hence, the generation of the symmetry can only be expected to occur as a limit of commutators of (not weakly converging) local charges.

It is worthwhile to stress that the non-invariance of the ground state expectation of a field F does not guarantee that one can write a corresponding Ward identity, a crucial ingredient for the Goldstone theorem.

The interplay between gauge invariance and the breaking of a continuous symmetry provides a mechanism for evading the conclusions of the Goldstone theorem, i.e. for allowing an energy gap in the presence of symmetry breaking.

In fact, let us consider the case in which

i) the continuous symmetry β^λ is defined by a (one-parameter) subgroup of the Heisenberg group G_H, which does not commute with the gauge transformations,

ii) in the ground state irreducible representation π of the observable algebra $\mathcal{A}$ there is a gauge invariant operator $F \in \pi(\mathcal{A})$, which yields a non-symmetric order parameter $< \delta F > \neq 0$, and
iii) the Hamiltonian is invariant under β^λ up to a time derivative which commutes with F,

then the conclusions of the Goldstone theorem do not apply by the following mechanism.

In the irreducible regular representation π_r of the field algebra $\mathcal{F}_W$, β^λ is implemented by a (weakly continuous) group of unitary operators $T(\lambda)$, all the matrix elements are invariant, but there is no gauge invariant (proper) vector state invariant under time translations. The symmetry gets broken by the direct integral decomposition of $\mathcal{H}_{\pi_r}$ over the spectrum of $\mathcal{Z}$, but one cannot write a symmetry breaking Ward identity for the expectation on the gauge invariant ground state.

On the other side, in the representation of $\mathcal{F}_W$ defined by a gauge invariant ground state ω_θ, the one-parameter group $T(\lambda)$ is not regularly represented. Therefore its generator cannot be defined as an operator in $\mathcal{H}_{\omega_0}$ and $\omega_\theta(\delta F) \neq 0$ cannot be written in terms of a limit of commutators of charges. In conclusion, the symmetry breaking Ward identity cannot be written in terms of expectations on θ states.

Such a mechanism is active in several quantum mechanics gauge models discussed in Chap. 3, as well as in the interesting case of chiral symmetry breaking in QCD, as discussed in Chap. 4.

4.5 Bloch Electron as a Gauge Model

The field algebra $\mathcal{F}_W$ is generated by the Weyl operators $U(\alpha)$, $V(\beta)$, $\alpha, \beta \in \mathbf{R}$ (we keep considering the one-dimensional case).

The periodic structure of the system leads to consider as observable C^*-algebra $\mathcal{A}$ the sub-algebra generated by $V(\beta)$ and by the periodic functions of the position $U(2\pi n/a)$, $n \in \mathbf{Z}$. The center $\mathcal{Z}$ of $\mathcal{A}$ is generated by the translations $V(a)$ and the irreducible representations of $\mathcal{A}$ are defined by the subspaces $\mathcal{H}_\theta$ (θ *sectors*).

The operators $U(\alpha/a), \alpha \neq 2\pi n$ intertwine between the inequivalent representations π_θ and $\pi_{\theta+\alpha}$ and the corresponding one-parameter group is non-regularly represented in the representation of $\mathcal{F}_W$ defined by the gauge invariant ground state Ψ_0.

The Bloch model has been discussed in order to clarify structures and mechanisms argued to characterize Quantum Chromodynamics (QCD).[12] For the analogies and correspondences we remark that the lattice translations $V(na)$ play the role of the large gauge transformations T_n and the θ sectors $\mathcal{H}_\theta$ correspond to the

[12] R. Jackiw, Topological Investigations of Quantized Gauge Theories, in S.B. Treiman, R. Jackiw, B. Zumino and E. Witten, *Current Algebra and Anomalies*, World Scientific 1985, p. 211–359, Sect. 3.5.

representations defined by the θ vacua, (here all the states $\Psi_\theta = U(\theta)\Psi_0$ have higher energy than Ψ_0). The transformations on $\mathcal{F}_W$ defined by the one-parameter group $\tilde{U}(\alpha) \equiv U(\alpha/a)$, $\alpha \in \mathbf{R}$: $\gamma_\alpha(F) \equiv \tilde{U}(\alpha)F\tilde{U}(\alpha)^{-1}$, $\forall F \in \mathcal{F}_W$, correspond to the chiral transformations.

The transformations γ_α are implemented by unitary operators in the space $\mathcal{H}$ carrying an irreducible representation of the (gauge dependent) field algebra $\mathcal{F}_W$; therefore they define Wigner symmetries there, but they do not leave the θ sectors invariant and therefore they are not implemented by unitary operators there. The corresponding symmetry is spontaneously broken in each θ sector.

An explicit symmetry breaking order parameter is provided by p or by $V(na)$, since $\gamma^\alpha(p) = p - \alpha$ and $(\Psi_\theta, \delta p\, \Psi_\theta) = \alpha \neq 0$. The Hamiltonian is invariant up to a time derivative:

$$\gamma^\alpha(H) = H - \alpha p/m.$$

The equations expected to hold in QCD are rigorously reproduced here

$$\tilde{U}(\alpha)\Psi_\theta = \Psi_{\theta+\alpha}, \quad V(na)\tilde{U}(\alpha)V(na)^{-1} = e^{i\alpha n}\,\tilde{U}(\alpha).$$

In the QCD context, the last equation is usually written in terms of the chiral charge Q^5, which is assumed to generate the chiral transformations,

$$T_n Q^5 T_n^{-1} = Q^5 + n,$$

however, it should be stressed that the generator of the "chiral" transformations does not exist, not only in the θ sectors, but not even in the large Hilbert space $\mathcal{H}$, because $\tilde{U}(\alpha)$ is non-regularly represented.

Thus, one cannot write a symmetry breaking Ward identity for the expectations on θ states. The overlooking of this subtle point is at the basis of problems and paradoxes affecting the use of Ward identities in the temporal gauge of QCD.

The Bloch model clearly displays the fact that the crucial ingredient for the breaking of chiral symmetry with energy gap (the so-called $U(1)$ problem) is the existence of a non-trivial center in the algebra of observables and its pointwise instability under chiral transformations.[13]

[13]For the realization and relevance of this structure see F. Strocchi, *Selected Topics on the General Properties of Quantum Field Theory*, World Scientific 1994, Sect. 7.4 and refs. therein; G. Morchio and F. Strocchi, J. Phys. A: Math. Theor. **40**, 3173 (2007); Ann. Phys. **324**, 2236 (2009).

5 Quantum Hall Electron: Zak States

The quantum mechanical behavior of an electron in a periodic lattice in the presence of a constant magnetic field is particularly interesting also in connection with the quantum Hall effect.

a) **Bloch electron in a constant magnetic field**

The Hamiltonian has the following form

$$H = \frac{\Pi^2}{2M} + W(\mathbf{x}), \quad \Pi_i \equiv p_i - \frac{e}{c} A_i, \quad i = 1, 2, 3, \tag{2.5.1}$$

where M denotes the electron mass and $W(\mathbf{x})$ is a bounded measurable periodic potential reflecting the lattice periodic structure in the $x\,y$ plane.

We adopt the symmetric gauge, so that the electromagnetic potential A_i is given by $A_i = -\frac{1}{2}\varepsilon_{ijk} H_j x_k$, we take the magnetic field $\mathbf{H}$ in the z-direction and consider the motion in the xy-plane. For simplicity, we shall use units such that $\hbar = 1 = M = e|\mathbf{H}|/c$, so that the cyclotron frequency $\omega_c = e|\mathbf{H}|/Mc$ and the magnetic length $l = (\hbar c/e|\mathbf{H}|)^{1/2}$ are both equal to one. Then, one has

$$\Pi_x = p_x - y/2, \quad \Pi_y = p_y + x/2, \quad [\,\Pi_y,\, \Pi_x\,] = i. \tag{2.5.2}$$

$\mathbf{\Pi}$ has the meaning of the (gauge invariant) velocity.

The lattice translations on the xy-plane are described by the operators

$$T(\mathbf{a}_j) \equiv e^{i\mathbf{\Pi}_c \cdot \mathbf{a}_j}, \quad j = 1, 2, \quad \mathbf{\Pi}_c \equiv \mathbf{p} + e\mathbf{A}/c, \tag{2.5.3}$$

$$[\,\Pi_{c\,x},\, \Pi_{c\,y}\,] = i, \quad [\,\mathbf{\Pi}_c,\, \mathbf{\Pi}\,] = 0, \tag{2.5.4}$$

where the vectors $\mathbf{a}_j$ are the lattice basis. The operators $T(\mathbf{a}_j)$, also called *magnetic translations*, commute with the Hamiltonian and satisfy the following commutation relation

$$T(\mathbf{a}_1)\, T(\mathbf{a}_2) = T(\mathbf{a}_2)\, T(\mathbf{a}_1)\, e^{i(a_{1\,x}\, a_{2\,y} - a_{1\,y} a_{2\,x})}. \tag{2.5.5}$$

Thus, they commute if the lattice cell satisfies the “rationality condition”[14]

$$a_{1\,x}\, a_{2\,y} - a_{1\,y}\, a_{2\,x} = 2\pi k, \quad k \in \mathbf{Z}. \tag{2.5.6}$$

In the following for simplicity we shall consider a square lattice with unit lattice spacing.

[14]For a detailed excellent discussion of the magnetic translation group see E. Brown, Aspects of Group Theory in Electron Dynamics, in *Solid State Physics*, F. Seitz et al. eds., Academic Press 1968, pp. 313–408.

The abelian group generated by the $T_j \equiv T(\alpha_j)$, with the condition of Eq. (2.5.6), will be denoted by $\mathcal{G}$. It plays the same role of the group of lattice translations $V(na)$ of the Bloch electron without magnetic field (see Sect. 4.5). It may therefore be given the meaning of an abelian *gauge group*.

In view of the above symmetry properties, it is convenient to describe the systems in terms of the two pairs of canonical (independent) variables

$$q \equiv \Pi_y, \quad p \equiv \Pi_x; \qquad Q \equiv \Pi_{cx}, \quad P \equiv \Pi_{cy}. \tag{2.5.7}$$

The corresponding Heisenberg group G_H is generated by the exponentials

$$u(\alpha) \equiv e^{i\alpha q}, \quad v(\beta) \equiv e^{i\beta p}; \qquad U(\gamma) \equiv e^{i\gamma Q}, \quad V(\delta) \equiv e^{i\delta P}.$$

We denote by $\mathcal{F}_W$ the corresponding *field C^*-algebra*. The elements $u(\alpha)$, $v(\beta)$, $U(n)$, $V(2\pi m)$ generate the *gauge invariant subgroup G_{obs}*, which can be interpreted as the observable subgroup. The corresponding C^*-algebra is denoted by $\mathcal{A}$, with the meaning of the *C^*-algebra of observables*. $\mathcal{A}$ has a non-trivial *center $\mathcal{Z}$* generated by the elements of the gauge group $\mathcal{G}$, which play the role of the large gauge transformations of QCD.

We start by considering the case of $W = 0$. In terms of the above canonical variables one has

$$H_0 = \tfrac{1}{2}(p^2 + q^2) = H_{osc} + \tfrac{1}{2}L_z, \tag{2.5.8}$$

$$H_{osc} \equiv \tfrac{1}{2}\,[p_x^2 + p_y^2 + \tfrac{1}{4}(x^2 + y^2)\,] = \tfrac{1}{4}\,(p^2 + q^2 + P^2 + Q^2), \tag{2.5.9}$$

$$L_z \equiv x p_y - y p_x = \tfrac{1}{2}(p^2 + q^2) - \tfrac{1}{2}(P^2 + Q^2). \tag{2.5.10}$$

L_z is conserved, but it does not commute with the gauge group $\mathcal{G}$ generated by the large gauge transformations $T_1 \equiv e^{i\sqrt{2\pi}Q}$, $T_2 \equiv e^{i\sqrt{2\pi}P}$.

The spectrum of H_0 is the familiar quantum oscillator spectrum, each level being now infinitely degenerate. For a very large magnetic field one may restrict the attention to the first Landau level (LL) corresponding to the lowest energy states of H. For the description of the degeneracy of the first LL one has many options.

One possibility, used for the discussion of Quantum Hall Effect, is to describe such a degeneracy in terms of eigenstates of L_z or of H_{osc}. With such a choice, a state (of the first LL) with maximum xy localization is

$$\Psi_{0\,0} \equiv (2\pi)^{-1/2} e^{-(x^2+y^2)/4}, \quad L_z \Psi_{0\,0} = 0$$

and it is also the ground state of the harmonic oscillator Hamiltonian $H_{osc}(Q, P) \equiv \frac{1}{2}(P^2 + Q^2)$.

A complete set of states for the first LL level if obtained by acting on $\Psi_{0\,0}$ by the magnetic translations

$$\Psi_{m\,n}(x, y) \equiv T(\mathbf{a}_1)^m\, T(\mathbf{a}_2)^n\, \Psi_{0\,0}(x, y).$$

Since, apart from (xy dependent phases) the magnetic translations act as lattice translations on the wave functions, the Ψ_{mn} defined above are peaked at the lattice points.

In this way, one gets a regular representation of the Heisenberg group G_H which, however, does not contain gauge invariant states, i.e. states invariant under the gauge group $\mathcal{G}$.

By an argument similar to that repeatedly used before (see e.g. Proposition 2.1) a *gauge invariant state* ω defines a non-regular representation of the Heisenberg group G_H (or of the exponential field algebra $\mathcal{F}_W$). Its representative cyclic vector Ψ_ω is an eigenstate of T_j

$$T_j\,\Psi_\omega = e^{i\theta_j}\,\Psi_\omega, \quad \theta_j \in [0, 2\pi), \quad j = 1, 2. \tag{2.5.11}$$

Such states are the so-called *Zak states*[15] $\omega_{\theta_1\,\theta_2}$

$$\begin{aligned}\omega_{\theta_1\,\theta_2}(U(\gamma)\,V(\delta)) &= e^{in\theta_1}\,e^{im\theta_2}, \quad \text{if} \ \ (\gamma, \delta) = \sqrt{2\pi}(n, m)\\ &= 0, \qquad\qquad\quad \text{if} \ \ (\gamma, \delta) \notin \sqrt{2\pi}(\mathbf{Z}, \mathbf{Z}).\end{aligned} \tag{2.5.12}$$

Clearly, the introduction of the periodic potential does not change such conclusions and actually strengthens the interpretation of the lattice translations as the generators of a gauge group, with a picture which is very close to the case of the Bloch electron without magnetic field. The first LL is not stable under the application of $u(\alpha)$, $v(\beta)$ and of the potential W.

As in case of zero magnetic field, the GNS representation space $\mathcal{K}$ defined by a gauge invariant state has an orthogonal decomposition over the spectrum of the generators of the gauge group

$$\mathcal{K} = \sum_{\theta_1,\,\theta_2} \oplus\, \mathcal{H}_{\theta_1,\,\theta_2}, \tag{2.5.13}$$

each $\mathcal{H}_{\theta_1,\,\theta_2}$ being the carrier of an irreducible representation of the gauge invariant algebra of observables $\mathcal{A}$.

The operators $U(\gamma)$, $V(\delta)$ intertwine between the θ sectors

$$U(\gamma)\,V(\delta)\,\mathcal{H}_{\theta_1,\theta_2} = \mathcal{H}_{\theta_1-\tilde{\delta},\,\theta_2+\tilde{\gamma}}, \qquad (\tilde{\gamma},\,\tilde{\delta}) \equiv \sqrt{2\pi}(\gamma, \delta).$$

They play the same role of the $U(\alpha)$ discussed in Sect. 4.5 and as such are the analogs of the chiral transformations in QCD; they commute with the Hamiltonian if the potential W (which plays the role of the fermion mass term in QCD) vanishes.

[15] J. Zak, Phys. Rev. **168**, 686 (1968).

They define Wigner symmetries in $\mathcal{K}$ which are broken in each irreducible representation $\mathcal{H}_{\theta_1,\theta_2}$ of the observable algebra. Such a breaking does not require the existence of Goldstone-like states by the same mechanism discussed in Sects. 4.3, 4.5.

The potential W is a periodic function of $x = q - P$ and $y = Q - p$ and since it commutes with T_j it must be a function of them[16] and therefore in each sector $\mathcal{H}_{\theta_1,\theta_2}$ it reduces to a periodic function of $q - \theta_2$, $Q - \theta_1$.

As in the case of vanishing magnetic field, in each θ sector W is infinitesimally smaller than $H_0 \equiv \frac{1}{2}(p^2 + q^2)$ in the sense of Kato; therefore, in each sector, since the spectrum of H_0 is discrete, so is the spectrum of $H = H_0 + W$, and, by a generalized Perron-Frobenius theorem as in the case of zero magnetic field (Sect. 3, Proposition 3.1), the ground state is unique. This implies that the spectrum of H is discrete in $\mathcal{K}$ and there is a (possibly degenerate) ground state in $\mathcal{K}$.

Particular instructive is the simple case of a periodic potential described by

$$W = \lambda \cos(\sqrt{2\pi}\, x)\, \cos(\sqrt{2\pi}\, y) = \lambda \cos(\sqrt{2\pi}(q - P)) \cos(\sqrt{2\pi}(Q - p)).$$

In the sector $\mathcal{H}_{\theta_1,\theta_2}$, W reduces to $\lambda \cos(\sqrt{2\pi} q - \theta_2) + \cos(\sqrt{2\pi} p - \theta_1)$ and to first order in λ the inf of the spectrum of H in $\mathcal{H}_{\theta_1,\theta_2}$ is

$$E_0(\theta_1, \theta_2) = \tfrac{1}{2} + \lambda e^{-\pi}\, (\cos(\theta_1) + \cos(\theta_2)). \tag{2.5.14}$$

Thus, for negative λ the minimum in $\mathcal{K}$ is obtained for $\theta_i = 0$, and for positive λ for $\theta_i = \pi$, $i = 1, 2$.

In conclusion one has

Proposition 5.1 *A gauge invariant state ω, i.e. a state invariant under magnetic translations, T_1, T_2, defines an irreducible representation $(\mathcal{H}_{\theta_1,\theta_2}, \pi_{\theta_1,\theta_2})$ of the observable algebra $\mathcal{A}$, labeled by the eigenvalues θ_1, θ_2 of the magnetic translations and non-regular representation $(\mathcal{K}, \pi)$ of the Heisenberg group G_H (and of the field algebra $\mathcal{F}_W$).*

The (non-separable) Hilbert space $\mathcal{K}$ has an orthogonal decomposition over the spectrum of the magnetic translations, Eq. (2.5.13).

The Hamiltonian H, Eq. (2.5.1), has a discrete spectrum in $\mathcal{K}$ and, at least for small periodic potential, a unique ground state belonging to the $\theta_1 = \theta_2 = 0$ sector.

It it worthwhile to remark that in the representation defined by a gauge invariant state the one-parameter groups of unitary operators $U(\gamma)$, $V(\delta)$ are not regularly represented, so that Q, P cannot be defined as operators in $\mathcal{K}$, only their exponentials exists in $\mathcal{K}$.[17]

[16] J. Zak, Phys. Rev. **168**, 686 (1968).

[17] With such a proviso, some of the paradoxes raised in the literature (see, e.g., R. Ferrari, Int. Jour. Mod. Phys. **12**, 1105 (1998)) disappear. In particular, the derivatives with respect to the angles θ_1, θ_2 correspond to the momenta canonically conjugated to Q, P respectively, and therefore cannot be defined in $\mathcal{K}$.

In our opinion, as in the case of zero magnetic field (Sect. 3), the description in terms of the representation given by the Hilbert space $\mathcal{K}$ clarifies the meaning and the role of the boundary conditions used in the literature for the wave function restricted to the primitive cell,[18] as a substitute of Eq. (2.5.11); such boundary conditions are unstable under the action of the unitary operators $U(\gamma)$, $V(\delta)$, which, instead, are well defined in $\mathcal{K}$. Thus, the description in terms of the states of $\mathcal{K}$ already takes the infinite volume limit into account.

b) **Quantum Hall electron**

In the Quantum Hall Effect (QHE) each electron lives in a periodic lattice under the influence of both a constant strong magnetic field, say in the z direction, and a constant electric field $\mathbf{E}$ in the xy plane.

It is convenient to choose the symmetric temporal gauge for the vector potential

$$A_i = -\tfrac{1}{2}\varepsilon_{ijk}H_j x_k - eE_i,$$

so that the motion of an electron in the xy plane is described by the following time dependent Hamiltonian

$$H(t) = \tfrac{1}{2}\tilde{\mathbf{\Pi}}^2 + W(\mathbf{x}), \qquad \tilde{\Pi}_i \equiv p_i - eA_i/c = \Pi_i - eE_i. \tag{2.5.15}$$

By means of a Galilei transformation[19] one can shift the dependence on the electric field from the "kinetic term" to the periodic potential, obtaining the following new Hamiltonian (by introducing the dual $\mathbf{E}^*$ of $\mathbf{E}$, $E_1^* \equiv -E_2$, $E_2^* \equiv E_1$)

$$H'(t) = \tfrac{1}{2}\Pi^2 + W(\mathbf{x} - e(\mathbf{E} + \mathbf{E}^* t)). \tag{2.5.16}$$

The only difference with respect to the case of zero electric field is that the periodic potential has become time dependent.

Thus, most of the previous analysis applies. In particular, the algebraic structure of the Heisenberg group G_H, of the exponential field algebra $\mathcal{F}_W$, of the gauge group $\mathcal{G}$ and of the gauge invariant or observable algebra $\mathcal{A}$ remain the same.

Gauge invariant states are analogously defined and the representations defined by them have the same properties as in Proposition 5.1.

[18]See, e.g. J. Zak, Phys. Rev. **168**, 686 (1968); E. Brown, Aspects of Group Theory in Electron Dynamics, in *Solid State Physics*, F. Seitz et al. eds., Academic Press 1968, pp. 313–408; F.D.M. Haldane, Phys. Rev. Lett. **55**, 2095 (1985).

[19]J. Belissard, Quantum systems periodically perturbed in time, in *Fundamental aspects of quantum theory*, V. Gorini and A. Frigerio eds., Plenum Press 1986, p. 163–171, and references therein; R. Ferrari, Int. Jour. Mod. Phys. **12**, 1105 (1998). For a comprehensive updated discussion of the quantum Hall effect and of the physical principles underlying it see: S. Bieri and J.M. Fröhlich, Comptes Rendus Physique, **12**, 332–346 (2011).

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