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Perfect Morse functions on compact manifolds of coherent states

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ABSTRACT : *Perfect Morse functions on the manifold of coherent states are effectively constructed. We consider the case of a compact, connected, simply - connected Lie group of symmetry, having the same rank as the stationary group of the manifold of coherent states. It is proved that the set of perfect Morse functions is dense in the set of energy functions for linear Hamiltonians in the elements of the Cartan algebra of the Lie algebra of the representation of the group considered. It is proved that the maximum number of orthogonal vectors on a coherent vector manifold is equal to the Euler-Poincaré characteristic of the manifold.*

1. *Introduction*

A particular attention has been paid lately to the application of geometrical ideas and methods in physics. Firstly, geometrical ideas, especially symplectic structures, have an important rol in classical mechanics [1]. Secondly, the geometry of classical phase space is the starting point of the geometrical quantization programme [17],[30]. On the other hand, the right application of the variational principles in quantum physics is conditioned on the establishment of the topological and global geometrical properties of quantum state manifolds [16].

Global variational methods are studied by means of the Morse theory. It is often useful to find the absolute minima of given functionals. In solving this difficult problem, Morse inequalities [23],[2],[21] can be used succesfully. Morse inequalities imply constraints on the stable and instable critical manifolds, imposed by the topology of the spaces on which the variational problems are considered. Morse inequalities have been applied to classical mechanics [24], Hartree-Fock problem [28],[5] , supersymmetry theories [33]. Atyah and Bott have applied Morse theory to determine the manifold of minima for the Yang-Mills functional in the equivariant case for Riemanian surfaces and gauge group $U(n)$ [2].

Morse inequalities become equalities for perfect Morse functions. The number of critical points of a given index of a perfect Morse function is minimal and is a topological invariant (the Batti number) of the manifold on which the variational problem is based. In the quantum case, many quantum states (e.g. the coherent [25],[26] state manifolds for Lie groups of symmetry) are obtained by embedding of some symplectic manifolds in Hilbert spaces of state vectors [27],[16]. Generally, these manifolds have locally phase space structure, but do not admit global canonical coordinates [1]. However, the corresponding quantum dynamical problems are global analysis problems. The perfect Morse functions just provide an economical method for the effective description of the geometry of quantum state manifolds. These functions exist only on manifolds without torsion [2], a fact verified long time ago for classical groups and G_2, F_4 [29].

In this paper, perfect Morse functions on a coherent state manifold are constructed for a compact, connected, simply-connected Lie group of symmetry, having the same rank as the stationary group of the manifold.

Sect. 2 comprises elements of Morse theory on manifold of quantum states: Morse inequalities and properties of perfect Morse functions. We limit ourselves to "Baby Morse theory", i.e. we do not refer to the equivariant Morse theory [2].

In Sect.3, perfect Morse functions are effectively constructed as energy functions associated to linear quantum systems, described by coherent state manifolds for Lie groups of symmetry. The cellular structure of these manifolds and the maximal orthonormal systems of coherent vectors are deduced.

Some applications to the Slater determinant manifold are outlined in Sect. 4. The last section is devoted to concluding remarks.

2. *Morse inequalities on manifold of quantum states*

1. The conventional model of quantum mechanics attaches to every physical system a complex Hilbert space $\mathcal{H}$. To every wave vector $\phi \in \mathcal{H}^* = \mathcal{H} \setminus \{0\}$ the state $\tilde{\phi} = \{ e^{i\varphi} \|\phi\|^{-1} \phi \mid \varphi \in \mathbb{R} \}$

is associated. The complex projective space of states is denoted by $\widetilde{\mathcal{H}}$.

Let $\xi : \mathcal{H}^* \to \widetilde{\mathcal{H}}$ be the projection $\xi(\phi) = \widetilde{\phi}$, $\phi \in \mathcal{H}^*$. The unitary sphere in $\mathcal{H}$ is defined as $\mathcal{S}(\mathcal{H}) = \{\psi / \psi \in \mathcal{H};\ \|\psi\| = 1\}$.

Let Q be a C^∞ - differentiable manifold [23] and let $\eta : Q \to \mathcal{S}(\mathcal{H})$ an injective and continuous mapping so that each function $f^\psi : Q \to \mathbb{C}$, $f^\psi(p) = \langle \psi, \eta(p) \rangle$, $p \in Q$, is differentiable. Here $\langle\ ,\ \rangle$ is the symbol of the scalar product of $\mathcal{H}$. The manifold $M = \eta(Q)$ is called *quantum vector manifold*. If the restriction of the projection ξ to M is injective, then $\widetilde{M} = \xi(M)$ is called *quantum state manifold*. The structure of differentiable manifold is canonically carried from Q onto M and $\widetilde{M}$.

Differentiable functions $f : M \to \mathbb{R}$ will be studied later. As a typical example, functions $f_A(\psi) = \langle \psi, A\psi \rangle$ will be considered in Sect.3, where $\psi \in M$ and A is a self-adjoint operator with M in the domain.

2. A brief review of Morse inequalities used further will be now outlined [23], [22], [2], [7]-[9], [5].

Let $f : M \to \mathbb{R}$ be a smooth function on a compact, C^∞, m-dimensional manifold M. The point $p \in M$ is a *critical point of f* if the tangent mapping vanishes at p, i.e., in a local system of coordinates of M, centred at p:

$$\partial f / \partial x_i |_p = 0, \quad i = 1, \ldots, m \tag{2.1}$$

The *Hessian* $H_p(f)$ at a critical point p is a well defined quadratic form on the tangent space to M, which, in a local system of coordinates, centred at p, relative to the base $(\partial/\partial x_1)_p, \ldots, (\partial/\partial x_m)_p$ is given by the matrix

$$H_p(f) = (\partial^2 f / \partial x_i \partial x_j)_p, \quad i, j = 1, \ldots, m. \tag{2.2.}$$

The number of negative (respectively zero) eigenvalues of the hessian matrix at a critical point p is called the *index* of p (the degeneracy degree, respectively), and is denoted by $\lambda_p(f)$. The critical point p is *non-degenerate* if its degeneracy degree is zero, i.e.

$$\det H_p(f) \neq 0. \tag{2.3}$$

A function $f : M \to \mathbb{R}$ with all the critical points non-degenerate is called a *Morse function*. The set of Morse functions on a compact manifold is an open set, dense in the set of differentiable functions on M (relative to the C^2 topology) [22].

Let $Cr(f)$ be the set of critical points of a Morse function f and let

$$C_q(f) = \sum_{p \in Cr(f)} \lambda_p(f), \quad \lambda_p(f) = q, \quad 0 \leq q \leq m. \tag{2.4}$$

The following (*Morse*) *inequalities are satisfied for the Morse functions*

$$C_\lambda(f) \geq b_\lambda, \qquad 0 \leq \lambda \leq m, \tag{2.5.1}$$

$$\sum_{i=0}^{\lambda} (-1)^{\lambda - i} C_i(f) \geq \sum_{i=0}^{\lambda} (-1)^{\lambda - i} b_i, \quad 0 \leq \lambda \leq m, \tag{2.5.2}$$

$$\sum_{i=0}^{m} (-1)^{m-i} C_i(f) = \sum_{i=0}^{m} (-1)^{m-i} b_i = \mathcal{X}(M), \tag{2.5.3}$$

where b_i is the i-th Betti number of M (relative to a field k, here real) and $\mathcal{X}(M)$ denotes the Euler-Poincaré characteristic of M.

Attaching to every Morse function f on M the *Morse-counter series*

$$M_t(f) = \sum_{p \in \mathcal{C}r(f)} t^{\lambda_p(f)} \tag{2.6.1}$$

$$M_t(f) = \sum C_i(f) t^i, \tag{2.6.2}$$

the Morse inequalities can be written compactly

$$M_t(f) - P_t(f) = (1+t) R(t), \tag{2.7}$$

where $R(t)$ is a polynomial with non-negative coefficients, and $P_t(M)$ is the Poincaré series for M.

A Morse function f satisfying the Morse inequalities (2.5.1) with the equal sign is called *a perfecte Morse function.* Note that if $C_{\lambda+1}(f) = C_{\lambda-1}(f) = 0$, then (2.5.2) implies $b_\lambda = C_\lambda(f)$, since, if $C_\lambda(f) = 0$ for every odd λ, then f is a perfect Morse function (*Morse lacunary principle*).

The connected submanifold $N \subset M$ is called *non-degenerate critical manifold for f* if and only if $N \subset \mathcal{C}r(f)$ and the restriction $H_N(f)$ of the Hessian to the normal bundle of N is non-degenerate. The latter condition means that, in a neighborhood of a point of N in which local coordinates $(x_1, \dots, x_n, x_{n+1}, \dots, x_m)$ on M ($n = \dim N$) can be chosen so that N is given locally by the equations $x_i = 0$, $i = n+1, \dots, m$, it is required that

$$H_N(f) = \det(\partial^2 f / \partial x_i \partial x_j)_{p \in N} \neq 0, \; i,j = n+1, \dots, m \tag{2.8}$$

A function f on M is called *non-degenerate (Morse) function in the extended sense* if $\mathcal{C}r(f)$ is a union of non-degenerate critical manifolds.

The number of negative eigenvalues of the Hessian (2.8) is called the index of N (relative to f) and is denoted by λ_N. The extended Morse series for the Morse function f is defined as

$$M_t(f) = \sum_{N \subset \mathcal{C}r(f)} t^{\lambda_N} P_t(N) \tag{2.9}$$

With this definition for $M_t(f)$, the Morse inequalities (2.7) persist for Morse functions in the extend sense. Let $\mathcal{C}r(f)$ be partitioned in classes N^μ with $d_{N^\mu,j}$ critical manifolds with the same j- Betti number, $j = 0, 1, \dots, m$. Then the coefficient $C_j(f)$ from (2.5) is given be [14]

$$C_j(f) = \sum_{N^\mu} \sum_{i=0}^{\min(\dim N^\mu, j)} b_i(N^\mu) d_{N^\mu, j-i} \tag{2.10}$$

and the extended Morse series (2.9) can be written as in eq. (2.6.2). So, the Morse function in the extended sense is perfect if in eq. (2.7) $R(t) \equiv 0$ and $M_t(f)$ is given by (2.9) or if inequalities (2.5.1.) are verified as equalities with $C_i(f)$ given by (2.10). *The Morse lacunary principle remains true for perfect Morse functions in the extended sense* [8].

3. *Construction of perfect Morse functions on compact manifold of coherent states*

1. Lately, the coherent states have been intensively studied [25], [26]. Now we shall introduce in a convenient manner the strictly necessary elements used in this paper.

A quantum system with symmetry (in the sense of Wigner [32] and Bargmann [3]) is characterized by a continuous homeomorphism $\tilde{\pi}$ of a topological group G into a group of transformations $\tilde{G}$ of the space $\tilde{\mathcal{H}}$ which leaves invariant the transition probabilities

$$((\tilde{\pi}(g)\tilde{\phi}, \tilde{\pi}(g)\tilde{\psi})) = ((\tilde{\phi}, \tilde{\psi})), \; g \in G, \; \tilde{\phi}, \tilde{\psi} \in \tilde{\mathcal{H}}, \tag{3.1}$$

where

$$((\tilde{\Phi}, \tilde{\Psi})) = \|\phi\|^{-1}\|\psi\|^{-1}|<\phi, \psi>|^2, \quad \phi, \psi \in \mathcal{H}^*.$$

Let $\tilde{\psi}_o \in \tilde{\mathcal{H}}$ be a fixed state. The $\tilde{G}$-orbit containing $\tilde{\psi}_o$

$$\tilde{M} = \tilde{G}\,\tilde{\psi}_o = \{\,\tilde{\pi}(g)\,\tilde{\psi}_o \mid g \in G\,\} \tag{3.2}$$

is called the ***manifold of coherent states***, and every $\tilde{\phi} \in \tilde{M}$ is called coherent state.

The closed group

$$K = \{\, h \mid h \in G \;;\; \tilde{\pi}(h)\tilde{\psi}_o = \tilde{\psi}_o \,\} \tag{3.3}$$

is also considered. Then $\tilde{\pi}(K)$ is a stationary group of the state $\tilde{\psi}_o$ and there exists the bijection $\tilde{\xi} = G/K \to \tilde{M}.$, defined by $\tilde{\xi}(g') = \tilde{\pi}(g)\tilde{\psi}_o$, where $g' = gK \in G|K$. Let the notation $\tilde{\xi}(g') = \tilde{\psi}(g')$. Evidently, $\tilde{\xi}(\vartheta') = \tilde{\psi}_o$, where ϑ is the unity element of the group G.

Further G will be taken a compact, connected, simply-connected Lie group. The manifold $\tilde{M}$ will be endowed with the canonical differentiable (even real analytic) structure induced by $\tilde{\xi}$ from the homogeneous space $G|K$, hence $\tilde{M}$ is a quantum state manifold diffeomorphic with $G|K$. On the other hand, according to a theorem of Wigner and Bargmann [32],[3], there exists a continuous, unitary representation π of the group G onto the complex Hilbert space $\mathcal{H}$, such that

$$\widetilde{\pi(g)\psi} = \tilde{\pi}(g)\,\tilde{\psi}\,;\quad g \in G, \quad \psi \in \mathcal{H}^*. \tag{3.4}$$

Then, there exists the cross section $\sigma : \tilde{M} \to \mathcal{S}(\mathcal{H})$ where σ is an injective mapping such that $\xi(\sigma(\tilde{\psi}(g'))) = \tilde{\psi}(g'), g' \in G|K$. Let the notations $M = \sigma(\tilde{M})$; $\psi(g') = \sigma(\tilde{\psi}(g'))$; $\psi_o = \sigma(\tilde{\psi}_o)$ .It follows that M is a differentiable manifold relative to the structure induced by σ from $\tilde{M}$. The manifold M is named ***coherent vector manifold***, and every $\phi \in M$ is called ***coherent vector***.

Let us also introduce the mappings $\xi_o : M \to \tilde{M}$ and $\eta : G|K \to M$ by $\xi_o(\psi(g')) = \tilde{\psi}(g') = \tilde{\xi}(g'), g' \in G|K$ and $\eta(g') = \sigma \circ \tilde{\xi}(g') = \sigma(\tilde{\psi}(g')) = \psi(g')$. Evidently, ξ_o, η and $\tilde{\xi} = \xi_o \circ \eta$ are diffeomorphisms. It follows that ***the coherent state manifold*** $\tilde{M}$, ***the coherent vector manifold*** M ***and the homogeneous space*** $G|K$ ***are diffeomorphic***. It can be noted that M is a system of coherent vectors of type (π, ψ_o) in the sense of Perelomov [25].

The previous construction is natural from the point of view of the interpretation of symmetries in quantum mechanics. Moreover, this construction is important for establishing the global properties of coherent state and coherent vector manifolds.

2. Further we need some elements of the theory of finite-dimensional representations of compact, connected, simply-connected Lie groups (see, for example [4],[15]). It will be sufficient to confine ourselves to groups whose complexification have complex, semi-simple Lie algebras. Indeed, the group G being compact, its Lie algebra is reductive. Moreover, the finite-dimensional representations of a semi-simple Lie algebra are completely reductive (Weyl), and any irreducible finite-dimensional representation is non-trivial only on the class of complex semi-simple Lie algebras.

Now, let T be a Cartan subgroup of the group G, and suppose that ψ_o is a j- dominant weight vector relative to the representation π. Let $\mathcal{H}_j$ denote the complex linear covering of the manifold M. Let π_j denote the restriction of the representation π to $\mathcal{H}_j$. Hence π_j is a finite-dimensional unitary irreducible representation of the group G onto the complex linear space $\mathcal{H}_j$. There exists an isomorphism π_j' of the Lie algebra $\mathfrak{g}$ of the group G onto the Lie algebra $\pi_j'(\mathfrak{g})$ of the group $\pi_j(G)$ such that

$$\pi_j(e^X) = \exp(\pi_j'(X)),\ X \in \mathfrak{g}, \tag{3.5.1}$$

where $e: \mathfrak{g} \to G$ and exp: $\pi_j'(\mathfrak{g}) \to \pi_j(G)$ are exponential mappings.

Let us also fix a Cartan-Weyl base [13] of the complexification $\mathfrak{g}^C$ of the Lie algebra $\mathfrak{g}$, with elements h_i, e_α, $1 \le i \le r$, $\alpha \in \Delta$, where r is the rank of the group G and Δ is a system of non-zero roots satisfying the commutation relations

$$[h_i, h_j] = 0, \quad [h_i, e_\alpha] = \alpha(h_i)e_\alpha, \tag{3.6.1}$$

$$[e_\alpha, e_{-\alpha}] = \sum_{i=1}^{r} \alpha(h_i)h_i, \tag{3.6.2}$$

$$[e_\alpha, e_\beta] = 0, \quad \alpha + \beta \notin \Delta \cup \{0\}, \tag{3.6.3}$$

$$[e_\alpha, e_\beta] = N_{\alpha\beta}e_{\alpha+\beta}, \quad \alpha + \beta \in \Delta, \tag{3.6.4}$$

where $1 \le i \le j \le r$, $\alpha, \beta \in \Delta$, and $\alpha(h_i)$, $N_{\alpha\beta}$ are real structure constants (cf. [13], pp 166-171). If $\alpha + \beta \neq 0$, then the roots e_α, e_β are orthogonal relative to the Killing form $B(\cdot,\cdot)$, and the relation $\alpha(h) = B(h, h_\alpha)$, where $h_\alpha = [e_\alpha, e_{-\alpha}]$ was taken into account in eq. (3.6.2). The root system Δ is included in the dual $\mathfrak{t}^*$ of the Cartan algebra $\mathfrak{t}$ of T, and by means of the mapping $\alpha \to h_\alpha$ Δ can be embedded in $\mathfrak{t}$.

The elements h_i $(1 \le i \le r)$ form a base of the complexification $\mathfrak{t}^C$ of the Cartan algebra $\mathfrak{t}$.

Let Π denote the set of simple roots. The simple roots can be chosen such that

$$\alpha_i(h_j) = \delta_{ij}, \quad \alpha_i \in \Pi,\ 1 \le i, j \le r \tag{3.7}$$

Every root $\alpha \in \Delta$ is a linear combination of simple roots from Π with integer coefficients of the same sign. If these coefficients are non-negative, the root α is called a positive root. Let Δ_+ denote the set of positive roots.

Let $\mathcal{C}$ be the fundamental Weyl chamber

$$\mathcal{C} = \{ w \mid w = \sum_{i=1}^{r} \lambda_i w_i,\ \lambda_i \in \mathbb{Z}_+ \}, \tag{3.8}$$

where the fundamental weights $w_i \in \mathfrak{t}^*$ verify the relations

$$2(w_i, \alpha_j) = \delta_{ij}(\alpha_j, \alpha_j), \quad 1 \le i, j \le r. \tag{3.9}$$

Here $(\ ,\ )$ denotes the Euclidean scalar product in $\mathfrak{t}^*$.

The representations π_j and π_j' can be uniquely extended to the group homomorphism $\pi_j^*: G^C \to \pi_j^*(G^C)$ and respectively, Lie algebra isomorphism, $\pi_j^{*\prime}: \mathfrak{g}^C \to \pi_j^{*\prime}(\mathfrak{g}^C)$ by

$$\pi_j^*(e^Z) = \exp(\pi_j^{*\prime}(Z)),\ Z \in \mathfrak{g}^C, \tag{3.5.2}$$

where $\pi_j^{*\prime}(\mathfrak{g}^C)$ is the complexification of the Lie algebra $\pi_j'(\mathfrak{g})$, but G^C and $\pi_j^*(G^C)$ denotes the complexification of the groups G and respectively $\pi_j(G)$. Of course, $\pi_j^*(G^C)$ and $\pi_j^{*\prime}(\mathfrak{g}^C)$ are sets of linear operators on $\mathcal{H}_j$. Let also the notations

$$H_i = \pi_j^{*\prime}(h_i),\ E_\alpha = \pi_j^{*\prime}(e_\alpha), \tag{3.10}$$

where $1 \le i \le r$ and $\alpha \in \Delta$. According to the theory of compact representations [4] the j-dominant weight can be chosen to belong to the Weyl chamber $\mathcal{C}$ and

$$\begin{aligned} H_i \psi_0 &= j_i \psi_0; && 1 \le i \le r, \\ E_{-\alpha} \psi_0 &\neq 0; && \alpha \in \Delta', \\ E_{-\alpha} \psi_0 &= 0; && \alpha \in \Delta \setminus \Delta', \end{aligned} \tag{3.11}$$

where $j = (j_1, \ldots, j_n)$ and

$$\Delta' = \{\not\mathcal{L} \mid \mathcal{L} \in \Delta ; (j, \mathcal{L}) < 0\} \tag{3.12}$$

We stress that in the present situation, the subspaces Δ' and $\Delta \setminus \Delta'$ can be chosen as *abelian subalgebras of* $\pi_j^*(\mathcal{g}^c)$ (cf [13], p.384).

The base of the real Lie algebra $\mathcal{g}$ (respectively $\pi_j'(\mathcal{g})$ is made of the elements ih_k, $i(e_{\mathcal{L}}+e_{-\mathcal{L}})$, $e_{\mathcal{L}}-e_{-\mathcal{L}}$ (respectively, the antihermitian operators iH_k, $i(E_{\mathcal{L}}+E_{-\mathcal{L}})$, $E_{\mathcal{L}}-E_{-\mathcal{L}}$, $1 \leq k \leq n$, $\mathcal{L} \in \Delta$).

Also, the unitarity of the representation π_j implies

$$H_i^+ = H_i, E_{\mathcal{L}}^+ = E_{-\mathcal{L}}, 1 \leq i \leq n, \quad \mathcal{L} \in \Delta, \tag{3.13}$$

where A^+ denotes the adjoint of the operator A.

Let $\mathcal{p}$ denote the complex Lie algebra with base $h_i, e_{\mathcal{L}}, 1 \leq i \leq n$, $\mathcal{L} \in \Delta \setminus \Delta'$. The complex Lie subgroup $P = e^{\mathcal{p}}$ of the group G^C is a parabolic group (Borel group, if $\Delta' = -\Delta_+$). The representation $\widetilde{\pi_j}$ is irreducible, $K = G \cap P$ and

$$P = \{g \mid g \in G^C ; \widetilde{\pi_j(g)\Psi_o} = \widetilde{\Psi_o}\} . \tag{3.14}$$

It follows that there is a diffeomorphism of homogeneous spaces $c : G/K \to G^C/P$, defined by $c(gK) = gP, g \in G$ [29].

Let $W(G)$ denote the Weyl group [13] associated with G, defined as the quotient $W(G) = N(T)/C(T)$ of the normalizer

$$N(T) = \{g \mid g \in G ; gTg^{-1} = T\} \tag{3.15}$$

of the Cartan group T by the corresponding centralizer $C(T) = \{g \mid g \in G \quad gt = tg , \text{ any } t \in T\}$. Similarly, $W(K)$ denotes the Weyl group associated with the group K. Let $\Sigma \subset N(T)$ be a set of elements such that the quotient space $W(G)/W(K)$ is made of the coset classes $(sC(T))W(K), s \in \Sigma$. Let us define the mappings $\widetilde{s} : \Delta \to \Delta$, for every $s \in \Sigma$, by

$$\widetilde{s}_{\mathcal{L}}(h) = \mathcal{L}(s^{-1} h s) , \quad h \in \Sigma , \quad \mathcal{L} \in \Delta . \tag{3.16}$$

The action of $\widetilde{s}_{\mathcal{L}}$ on an element k of the space generated by Δ is the reflection

$$\widetilde{s}_{\mathcal{L}}(k) = k - 2(\mathcal{L}, k)\mathcal{L}/(\mathcal{L}, \mathcal{L}), \tag{3.17}$$

and for every $\mathcal{L} \in \Delta$, there exists $\beta \in \Pi$ and $\gamma \in \Delta$ such that $\mathcal{L} = \widetilde{s}_{\beta}(\gamma)$.

3. With the previous facts, the Kählerian structure of the homogeneous space G^C/P will be carried onto the manifold M of coherent vectors. Moreover, the Kählerian structure of the homogeneous space G^C/P will be also transported onto the homogeneous space G/K. Note also that the group K is still a connected group, with the same rank as G [29].

Let the vectors

$$\Phi_z = \exp\left(\sum_{\mathcal{L} \in \Delta'} z_{\mathcal{L}} E_{-\mathcal{L}}\right)\Psi_o, \tag{3.18}$$

$$\Psi_z = \|\Phi_z\|^{-1} \Phi_z = \Psi(g'), \tag{3.19}$$

for

$$c(g') = \exp\left(\sum_{\mathcal{L} \in \Delta'} z_{\mathcal{L}} E_{-\mathcal{L}}\right)P, \tag{3.20}$$

where z belongs to the m-dimensional Euclidean complex space $\mathbb{C}^m$ and

$$2m = \dim \widetilde{M} = \dim M = \dim G/K = \dim G^C/P . \tag{3.21}$$

Let the notation

$$\mathcal{V}_o = \{ \psi_z \mid z \in \mathbb{C}^m \}$$

and let us consider the homeomorphism h: $\mathcal{V}_o \to \mathbb{C}^m$, defined by $h^{-1}(z) = \psi_z$. Let also the notation $\mathcal{V}_s = \mathcal{T}_j(s)\mathcal{V}_o$ and $h_s = h \circ \mathcal{T}_j(s)^+$ for every $s \in \Sigma$. Then $(\mathcal{V}_s)_{s\in\Sigma}$ *is an open, finite covering of the manifold M, and the collection of local charts* $(\mathcal{V}_s, h_s)_{s\in\Sigma}$ *generates and atlas of a Kahlerian manifold* [27] *with the fundamental 2- form on* $\mathcal{V}_o$

$$\omega = -i \sum_{\alpha,\beta\in\Delta} g_{\alpha\bar\beta}\, dz_\alpha \wedge d\bar z_\beta \,,$$

where

$$g_{\alpha\bar\beta} = \partial^2 F(z,\bar z)/\partial z_\alpha\, \partial\bar z_\beta \,, \tag{3.22}$$

$$F(z,\bar z) = \ln \langle \Phi_z , \Phi_z \rangle . \tag{3.23}$$

The Kahlerian structure of the mainofld M is induced by the mapping ξ_o *onto the coherent state manifold* $\tilde M$.

To every linear operator A on $\mathcal{H}_j$, a function $f_A : \tilde M \to \mathbb{C}$ can be associated by

$$f_A(\tilde\psi) = \langle \psi, A\psi \rangle ; \quad \psi \in M , \tag{3.24}$$

called the *covariant symbol* [8]. If A is a Hermitian operator associated to an observable, then f_A is a real function, and $f_A(\tilde\psi)$ can be interpreted as expectation value of the considered observable. If H is a Hamiltonian, then f_H is called an energy function. The manifold $\tilde M$ being Kählerian, is of course also symplectic, hence the symbol f_A associated to a Hermitian operator admits the interpretation of a classical observable.

Let us now introduce the notation

$$\lambda_\alpha = \sum_{i=1}^{r} \varepsilon_i\, \alpha(H_i) , \quad \varepsilon = (\varepsilon_1, \dots, \varepsilon_r) \in \mathbb{R}^r . \tag{3.25}$$

After this long preparation, we are ready to state the main theorem of the paper.

<u>*Theorem 1*</u>. *The energy function* f_H *associated to the Hamiltonian*

$$H = \sum_{i=1}^{r} \varepsilon_i H_i \,, \quad \varepsilon = (\varepsilon_1, \dots, \varepsilon_r) \in \mathbb{R}^r \tag{3.26}$$

is a perfect Morse function in the extended sense.

Moreover if

$$\lambda_{\tilde s_\alpha} \neq 0 , \quad s \in \Sigma , \quad \alpha \in \Delta' , \tag{3.27}$$

then the associated energy function f_H *is a perfect Morse function.*

<u>*Proof*</u>. Let us consider the function f: $\mathbb{C}^m \to \mathbb{R}$ defined by

$$f(z,\bar z) = \langle \psi_z , H\psi_z \rangle ; \quad z \in \mathbb{C}^m . \tag{3.28}$$

The function f can be put into the form

$$f(z,\bar z) = \sum_{i=1}^{r} \varepsilon_i\, j_i - \sum_{\gamma\in\Delta'} \lambda_\gamma\, z_\gamma\, \partial F(z,\bar z)/\partial z_\gamma . \tag{3.29}$$

Indeed, from eqs. (3.18) and (3.19) it follows that

$$f(z,\bar z) = \|\Phi_z\|^{-2} \langle \Phi_z , H e^X \psi_o \rangle , \tag{3.30}$$

where X denotes

$$X = \sum_{\alpha\in\Delta'} z_\alpha E_{-\alpha} \tag{3.31}$$

But

$$He^{X}=e^{X}\sum_{n\geq 0}(n!)^{-1}(-\mathrm{ad}X)^{n}H=e^{X}(H-[X,H]+1/2[X,[X,H]]+\dots). \qquad (3.32)$$

From (3.11) and (3.26) it results

$$H\psi_0=\sum_{i=1}^{n}\varepsilon_i\, j_i\, \psi_0 \qquad (3.33)$$

and, combining eqs (3.26), (3,31), (3.6.1) and (3.25) we get

$$[X,H]=\sum_{\alpha\in\Delta'} z_\alpha \lambda_\alpha E_{-\alpha}\ , \qquad (3.34)$$

$$[X,[X,H]]=0 \qquad (3.35)$$

From the relations (3.32) - (3.35), we get

$$He^{X}\psi_0=e^{X}\Big(\sum_{i=1}^{n}\varepsilon_i j_i-\sum_{\alpha\in\Delta'} z_\alpha\lambda_\alpha E_{-\alpha}\Big)\psi_0$$

Introducing the latter expression in eq. (3.30) and taking into account eq. (2.23), the relation (3.29) is proved.

The point $z\in\mathbb{C}^m$ is a critical point of the function f if and only if

$$\partial f/\partial\bar{z}^{\beta}=-\sum_{\gamma\in\Delta'}\lambda_\gamma z_\gamma\ \partial^2F/\partial z_\gamma\,\partial\bar{z}_\beta=0,\ \beta\in\Delta'. \qquad (3.36)$$

Since the fundamental 2-form ω is non-degenerate, the matrix $\Gamma=(g_{\gamma\bar\beta})_{\gamma,\beta\in\Delta'}$ is non-singular. Then equation (3.36) is equivalent to the conditions

$$\lambda_\gamma z_\gamma=0\ ;\qquad \gamma\in\Delta'. \qquad (3.37)$$

The manifold of critical points of f is

$$Cr\, f=\{z\ |\ z\in\mathbb{C}^m;\ z_\gamma=0,\ \gamma\in\Delta''\}, \qquad (3.38)$$

where

$$\Delta''=\{\gamma\ |\ \gamma\in\Delta';\ \lambda_\gamma\neq 0\} \qquad (3.39)$$

If the point $z_0\in Cr(f)$, then (3.36) and (3.37) imply

$$(\partial^2 f/\partial z_\alpha\,\partial z_\beta)_{z_0}=(\partial^2 f/\partial\bar{z}_\alpha\,\partial\bar{z}_\beta)_{z_0}=0,\ \alpha,\beta\in\Delta'; \qquad (3.40)$$

$$(W_{z_0}(f))_{\alpha\beta}=(\partial^2 f/\partial z_\alpha\,\partial\bar{z}_\beta)_{z_0}=-\lambda_\alpha g_{\alpha\bar\beta}=-g_{\alpha\bar\beta}\,\lambda_\beta\,. \qquad (3.41)$$

From eq.(3.41) it results that the positive definite matrix Γ and the matrix $\Lambda=(\lambda_\alpha\delta_{\alpha\beta})_{\alpha,\beta\in\Delta'}$ are simultaneously diagonalizable. So, the Hessian matrix of the function f in z_0

$$H_{z_0}(f)=2U\begin{pmatrix}W&0\\0&W^t\end{pmatrix}U^{+},\ U=2^{-1/2}\begin{pmatrix}\mathbb{1}_m&\mathbb{1}_m\\ i\mathbb{1}_m&-i\mathbb{1}_m\end{pmatrix} \qquad (3.42)$$

admits λ_- (respectively λ_0) negative (respectively zero) eigenvalues, where

$$\lambda_-=2\,card\,\{\gamma\ |\ \gamma\in\Delta';\ \lambda_\gamma>0\},$$

$$\lambda_0=2\,card\,\{\gamma\ |\ \gamma\in\Delta';\ \lambda_\gamma=0\}, \qquad (3.43)$$

and $\mathbb{1}_n$ denotes the unit matrix of the group $GL(n,\mathbb{C})$ and W^t denotes the transpose of the matrix W. In eq. (3.42) the Hessian is expressed in the real coordinates (x_α, y_α), where $z_\alpha=x_\alpha+iy_\alpha$;

$$(H(f))_{\alpha\beta}=\begin{pmatrix}\partial^2 f/\partial x_\alpha\partial x_\beta & \partial^2 f/\partial x_\alpha\partial y_\beta\\ \partial^2 f/\partial y_\alpha\partial x_\beta & \partial^2 f/\partial y_\alpha\partial y_\beta\end{pmatrix};\ \alpha,\beta\in\Delta'. \qquad (3.44)$$

The eqs.(3.39) - (3.43) imply that the Hessian matrix (3.44) has non-zero determinant $\det(H(f))_{\alpha,\beta\in\Delta'}\neq 0$, hence the manifold (3.38) is a non-degenerate critical manifold. A point (vector) of this manifold has the expression

$$\psi_{z,cr}=\exp\Big(\sum_{\alpha\in\Delta'\setminus\Delta''} z_\alpha E_{-\alpha}\Big)\psi_0 \qquad (3.45)$$

Now, choosing $f^{s} = f_H \circ \xi_0 \circ \mathcal{T}_j(s) \circ h^{-1}$, $s \in \Sigma$, it follows that the non-degenerate critical manifolds of $\widetilde{M}$ for f^{s} are described by $\widetilde{\psi}^{s}_{z,cr}$ where $\widetilde{\psi}^{s}_{z,cr} = \widetilde{\mathcal{T}_j(s)\psi_{z,cr}}$. Every non-degenerate critical manifold has even index

$$\lambda_{s,cr} = 2\,card\{\mathcal{L} \mid \mathcal{L} \in \Delta''; \lambda_{\widetilde{\Lambda}_{\mathcal{L}}} > 0\}. \qquad (3.46)$$

It follows that in eq. (2.9) the fiber of the non-degenerate critical manifold has even dimension, and, moreover, the coefficients $C_i(f)$ (2.10) are all even, hence the lacunary principle of Morse in the extended sense is applicable.

The fist part of Theorem 1 was proved.

If $\Delta' = \Delta''$, then $z_0 = 0$ is the only critical point of the function f. This point is a non-degenerate one and has an even index (3.43).

If the conditions (3.27) are fulfiled, then it results that the critical points of the function f_H are the distinct states $\widetilde{\psi}^{s}$, $s \in \Sigma$, where $\psi^{s} = \mathcal{T}_j(s)\psi_0$. Every critical state $\widetilde{\psi}^{s}$ is non-degenerate and has an even index

$$\lambda_s = 2\,card\{\mathcal{L} \mid \mathcal{L} \in \Delta'; \lambda_{\widetilde{\Lambda}_{\mathcal{L}}} > 0\}. \qquad (3.47)$$

Now, the lacunary principle of Morse is applied and the Theorem is proved.

__Remark 1__. The set of perfect Morse functions is dense in the set of energy functions associated to Hamiltonians which are linear in H_i, $i = 1,\dots, r$.

__Remark 2__. The Theorem is also true for Hamiltonians H such that iH belongs to the Lie algebra $\mathcal{T}_j'(\mathfrak{g})$.

As a direct application of Theorem 1, a description follows of the maximal orthogonal system of coherent vectors.

__*Theorem 2*__. *If $\mathcal{T} \subset M$ is a maximal orthogonal system of coherent vectors, then there exists an element $g \in G$ such that*

$$\mathcal{T} = \{\mathcal{T}(g)\psi^{s} \mid s \in \Sigma\} \qquad (3.48)$$

and the number of vectors in $\mathcal{T}$ is equal to the Euler-Poincaré characteristic $\chi(M)$.

__*Proof*__. The perfect Morse function f_H appearing in Theorem 1 induces a cellular structure onto the manifold of coherent states $\widetilde{M}$. For every $s \in \Sigma$ there exists in the cell $\widetilde{\mathcal{V}}_s = \xi(\mathcal{V}_s)$ one and only one critical state $\widetilde{\psi}^{s}$ of the function f_H. Observing that $\{\widetilde{\mathcal{V}}_s\}_{s\in\Sigma}$ is an open covering of the manifold $\widetilde{M}$, that the group $\widetilde{G}$ acts transitively on M, and that

$$\langle \psi^{s}, \psi^{s'} \rangle = \delta_{ss'}, \quad \langle \psi_0, \psi_z \rangle \neq 0, \qquad (3.49)$$

for $s, s' \in \Sigma$, $z \in \mathbb{C}^m$, eq. (3.48) follows. On the other hand, from the Morse equality (2.5.3.) with all odd Betti numbers equal to zero, it can be deduced that Σ and $\mathcal{T}$ have exactly $\chi(M)$ elements.

4. Applications to the manifold of Slater determinats

From the precedent section, it can be noted that the results outlined there are applicable to large classes of quantum systems with symmetry, where G is compact and $\mathrm{rank}G = \mathrm{rank}K$. The situation is reducible to quantum state manifolds diffeomorphic with the irreducible Hermitian symmetric spaces ($SU(p+q)/S(U(p)\times U(q))$, $SO(2n)/U(n)$, $SO(p+2)/SO(p)\times SO(2)$, $Sp(n)/U(n)$ and two special cases, cf.ref.[13], pp.518). With this observation, the previous results are effectivly applicable to problems with variational principles on coherent state manifolds, and particularly to Hartree-Fock and Hartree-Fock-Bogoliubov principles.

Here we sketch a short application of the general Theorem 1 to the Hartree-Fock case. Details will be presented elsewhere.

The time-dependent variational principle of Hartree-Fock is based on the Slater determinant manifold [11]. A geometrical description of this manifold will be achieved by means of perfect Morse functions and topological constraints onto the energy function will also be established.

Let us consider a fermion Fock space $\mathcal{H}$ with vacuum state $\hat{\Omega}$. Let $\mathcal{H}_j$ denote the linear complex subspace of $\mathcal{H}$ with a base formed by the n-particle vectors

$$a^+_{p_1} a^+_{p_2} \cdots a^+_{p_n} \Omega \quad ; \quad 1 \leq p_1 < p_2 \cdots < p_n \leq n', \tag{4.1.}$$

where a^+_p, a_p ($p = 1, \ldots, n'$) are the usual fermion creation and annihilation operators respectively.

The Hartree-Fock Hamiltonian is a Hermitian operator on $\mathcal{H}_j$, realized as a second degree polynomial in bi-fermion operators

$$C_{pq} = a^+_p a_q \quad ; \qquad 1 \leq p,q \leq n' . \tag{4.2}$$

From the usual anti-commutation relations of the annihilation and creation operators, it follows

$$[C_{pq}, C_{p'q'}] = \delta_{qp'} C_{pq'} - \delta_{pq'} C_{qp} \; ; \; 1 \leq p,q \leq n'. \tag{4.3}$$

The Lie algebra of antihermitian operators on $\mathcal{H}_j$, which are linear combinations with complex coefficients x_{pq}, $x_{pq} = -\bar{x}_{qp}$ of the operators C_{pq}, is isomorphic with the Lie algebra $u(n')$ of the group $U(n')$. But the group $U(n')$ is canonically isomorphic with the product of groups $U(1) \times SU(n')$, being of course connected, simply-connected. Hence, it can be chosen that $G = SU(n')$. Let us also fix the initial vector

$$\psi_0 = a^+_1 a^+_2 \cdots a^+_n \Omega \tag{4.4}$$

Since

$$\begin{aligned} C_{pq} \psi_0 &= \delta_{pq} \psi_0 \; ; \quad 1 \leq p,q \leq n \; ; \\ C_{pq} \psi_0 &= 0 \quad ; 1 \leq p \leq n \; ; \; n+1 \leq q \leq n', \\ C_{pq} \psi_0 &\neq 0 \quad ; n+1 \leq p \leq n', \; 1 \leq q \leq n , \end{aligned} \tag{4.5}$$

ψ_0 is a vector of dominant weight $j = (1^n \; 0^{n'-n})$ of the unitary irreducible representation π_j of $SU(n')$ on $\mathcal{H}_j$.

A manifold of coherent states of dimension $m = 2n(n'-n)$ is obtained

$$\tilde{M} = \{ \tilde{\Psi} \mid \tilde{\Psi} = \widetilde{\pi_j(g) \psi_0} \; ; \; g \in SU(n') \}, \tag{4.6}$$

and is diffeomorphic with the complex Grassmann manifold $G_n(\mathbb{C}^{n'}) \approx U(n') / U(n) \times U(n'-n)$ [10],[5]. The manifold of coherent vectors M is diffeomorphic with $\tilde{M}$, as in Sect.3. Here we introduce the notations

$$\begin{aligned} \Phi_Z &= \exp\Big(\sum_{p=n+1}^{n'} \sum_{q=1}^{n} \bar{z}_{qp} \, C_{qp} \Big) \psi_0 , \\ \Sigma &= \{ \Delta^\sigma \mid \sigma \in S(n, n') \} , \\ \Delta^\sigma &= (\delta_{i \, \sigma(j)})_{1 \leq i, j \leq n'} , \end{aligned} \tag{4.7}$$

where $Z = (z_{pq})_{n+1 \leq p \leq n', \, 1 \leq q \leq n} \in \mathbb{C}^{n(n'-n)}$ and the set $S(n, n')$ of $C_n^{n'}$ Schubert symbols comprises all permutations $\sigma : \{1, 2, \ldots, n'\} \rightarrow \{1, 2, \ldots, n'\}$ with the property that its restrictions to the subsets $\{1, 2, \ldots, n\}$ and $\{n+1, \ldots, n'\}$ are increasing. The atlas of the manifold M is generated by the open covering $\{ \mathcal{V}_\sigma \}_{\sigma \in S(n,n')}$ where

$$\mathcal{V}_\sigma = \{ \pi_j(\Delta^\sigma) \, \psi_Z \mid Z \in \mathbb{C}^{n(n'-n)} \} . \tag{4.8}$$

Here the local coordinate mappings $h_\sigma : \mathcal{V}_\sigma \rightarrow \mathbb{C}^{n(n'-n)}$ are

$$h_\sigma(\psi_{Z\sigma}) = Z , \quad \pi_j(\Delta^\sigma)^+ \psi_{Z\sigma} = \psi_Z \; ; \quad \sigma \in S(n, n') . \tag{4.9}$$

The manifold M is called the *Slater determinant manifold* (in the second quantization).

According to Theorem 1, *the energy function* f_{H_0} *associated to the Hamiltonian*

$$H_0 = \sum_{i=1}^{n} c_i \, C_{ii} \quad , \quad c_1 < c_2 < \ldots < c_n , \qquad (4.10)$$

is a perfect Morse function.

By direct calculation [5] it is obtained for $f = f_{H_0} \circ \xi \circ \mathcal{T}_{\Omega}(\Omega^{\sigma})^{-1}$

$$\begin{aligned} f(Z) &= Tr\,[(U + Z V Z^+)(\mathbb{1}_n + Z Z^+)^{-1}], \\ U &= (c_p \delta_{pq})_{1 \le p, q \le n} \, , \\ V &= (c_p \delta_{pq})_{n+1 \le p, q \le n'} \, . \end{aligned} \qquad (4.11)$$

Then, the function $f : \mathbb{C}^{n(n'-n)} \to \mathbb{R}$ has an unique critical point $Z = 0$. This point is non-degenerate, and the Hessian matrix has double degenerate eigenvalues: $c_q - c_p \; ; \; 1 \le p \le n < q \le n'$.

The critical set of the energy function f_{H_0} consists of the critical states $\Psi_\sigma \; (\sigma \in S(n, n'))$, where

$$\psi_\sigma = a^+_{\sigma(1)} a^+_{\sigma(2)} \cdots a^+_{\sigma(n')} \, \Omega \, , \qquad (4.12)$$

and the critical state Ψ_σ has the index

$$\lambda_\sigma = 2\, card\{(p,q) \,|\, 1 \le p \le n < q \le n' ; \sigma(p) > \sigma(q)\}. \qquad (4.13)$$

It is funny to recover directly the Betti numbers of the manifold M of Slater determinants

$$\begin{aligned} b_{2\lambda+1} &= 0 \; ; \; 0 \le \lambda \le n(n'-n); \\ b_{2\lambda} &= card\{(\omega_1, \ldots, \omega_n) \in \mathbb{Z}^n_+ \,|\, 0 \le \omega_1 \le \ldots \le \omega_n \le n'-n; \\ & \qquad \omega_1 + \omega_2 + \ldots + \omega_n = \lambda\}, \end{aligned} \qquad (4.14)$$

and also the Euler-Poincaré characteristic $\chi(M) = C_n^{n'}$.

<u>Remark 3.</u> Observing that the uni-particle states are eigenstates with eigenvalues c_i, i = 1, ..., n, it can be noted that perfect Morse functions are obtained when the uni-particle space is non-degenerate.

<u>Remark 4.</u> If the Hartree-Fock energy function f_H admits only non-degenerate critical sets then the Morse inequalities (2.5) are satisfied, where $0 \le \lambda \le m = 2n(n'-n)$, $C_\lambda(f)$ is the number of critical states of index λ for f_H and the Betti numbers are given by (4.14). The problem of existence of Hartree-Fock states for Hamiltonian which do not have spurious states was analysed in ref. [28]. The Hamiltonian which gives the minimum number of Hartree-Fock states was here effectively constructed. It can also be shown that if the eigenvalues of the uni-particle states c_i are not all distinct, then the set of critical sets are Grassmann submanifolds of the Grassmann manifold.

5. *Conclusion and discussion*

The Morse inequalities in classical and extended sense have been used for the effective construction of perfect Morse functions on manifold of quantum states and quantum vectors. Actually, the case of a compact Lie group was considered. It was proved that the set of perfect Morse functions is dense in the set of energy functions for linear Hamiltonians in the elements of the Cartan algebra of the Lie algebra of the representation of the considered group, which was chosen compact, connected, simply-connected and having the same rank as the stationary group of the manifold of coherent states. By the construction of perfect Morse functions, the cellular decomposition of the manifold of coherent states was found. For every energy function, the Morse inequalities are satisfied, the odd Betti numbers being in this case zero. Particularly, the energy function admits a number of critical points at least equal to the Euler-Poincaré characteristic of the manifold of coherent states. It is also proved that the Euler-Poincaré characteristic is equal to the maximum number of orthogonal vectors.

The results obtained permit a correct approach to different problems of classical limit and variational principles on manifold of coherent states from the point of view of global analysis and geometry. In this context, the cellular decomposition of coherent state manifolds induced by the perfect Morse functions is useful for solving assymptotical problems of actual interest such as: the classical limit of quantum collective models [20],[31], 1/N expansions in quantum field theory [6], semi-classical behaviour of functional integral based on coherent states [34], Lagrangian analysis [19] and the connection between the geometric quantization method and the functional integral [12].

An extended version of this paper is in preparation.

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