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Curvature of the Slater determinant manifold

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Résumé. — L'application d'une droite de l'espace particule-trou dans la variété des déterminants de Slater engendre une trajectoire de courbure comprise entre 1 et $\sqrt{3}$. Cette courbure dépend de la direction de la droite, ce qui rend l'espace particule-trou anisotrope. Des résultats préliminaires indiquent que les mouvements collectifs induisent des chemins de courbure plus forte que les mouvements non collectifs.

Abstract. — The mapping of a straight line in the particle-hole space onto the manifold of Slater determinants is found to induce a trajectory whose curvature is between 1 and $\sqrt{3}$. This curvature depends on the direction of the line, which renders the particle-hole space anisotropic. There are indications that collective motion induces a large curvature of the path.

1. **Introduction.** — Slater determinants are very often used as first approximations to the microscopic wave functions of an N -body nuclear system. This is due, of course, to the simplifications they introduce in practical calculations but also to the possibility of parametrization of these determinants by simple physical quantities (orientations, deformations...), to the corresponding formulation of nuclear dynamics in terms of average potentials when collective processes are involved, and finally to the natural hierarchy of particle-hole excitations when non collective degrees of freedom must be reinstated. The Hartree-Fock, constrained Hartree-Fock and time-dependent Hartree-Fock theories of course make great use of Slater determinants. The shell model, the generator coordinate theory and several other theories also use linear combinations of these determinants as well.

It is thus of some interest to analyse whether Slater determinants Φ give a flexible [1-4] set of trial functions. This question must be distinguished from the fact that Hartree-Fock Hamiltonians and equations are non linear with respect to Φ , which is more of a dynamical problem. We are rather concerned with the well-known fact that a linear combination of determinants is not a determinant in general, a feature which has been noticed and discussed by many authors.

The general interpretation which is given for this special non-linearity is that Hartree-Fock theories are close to the limit of classical mechanics (and one must reinstate the superposition principle at a later stage). The present work actually intends to present a geometrical image of the non-linearity of Slater determinants.

This image consists in considering first the sphere of arbitrary wave functions Ψ normalized to unity in the Hilbert space. The set S of Slater determinants normalized to unity is a subset of this sphere. Two normalized and orthogonal determinants Φ and Φ' can be connected by a path on the sphere, made of the wave functions $\Psi = \cos \theta \Phi + \sin \theta \Phi'$ where θ is an arbitrary real angle. This path can be called a meridian circle. Its radius of curvature is obviously equal to 1. The point is that this path goes out of the set S in general. Even if one takes Φ and Φ' to be non-orthogonal to each other, the only way to remain on S is to connect Φ and Φ' through transformations of the kind $\exp(iA)$, where A is a one-body operator. As will be seen in the following, the paths defined by such transformations will have in general a curvature larger than 1.

Section 2 of this paper gives a brief review of how one can define the curvature of a path in a Hilbert space. Section 3 gives an illustrative example of the theory and section 4 contains a more general result. A discussion and a conclusion are proposed in section 5.

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2. Definition of curvature. — One might attempt to consider S as a Riemannian manifold and define covariant derivatives, Christoffel symbols and a global curvature tensor. For the more limited purpose of the description of a path $\Psi(\lambda)$, where λ is a real parameter, it is much simpler to calculate the curvature of the path itself. This only requires the existence of the first two derivatives : $d\Psi/d\lambda$ and $d^2\Psi/d\lambda^2$ and the assumption that these two derivatives are square integrable vectors.

The length element dl along the path is then defined by

$$\frac{dl}{d\lambda} = \left[\left\langle \frac{d\Psi}{d\lambda} \middle| \frac{d\Psi}{d\lambda} \right\rangle \right]^{1/2}, \quad (1)$$

and the unit tangent vector $|T\rangle$ along the path is

$$|T\rangle = \left(\frac{dl}{d\lambda} \right)^{-1} \left| \frac{d\Psi}{d\lambda} \right\rangle. \quad (2)$$

The unit, main normal vector $|N\rangle$ and the curvature C along the path are then defined by

$$C|N\rangle = \left| \frac{dT}{d\lambda} \right\rangle = \left[\left| \frac{d^2\Psi}{d\lambda^2} \right\rangle - \left| \frac{d\Psi}{d\lambda} \right\rangle \left(\frac{dl}{d\lambda} \right)^{-2} \times \right. \\ \left. \times \operatorname{Re} \left\langle \frac{d\Psi}{d\lambda} \middle| \frac{d^2\Psi}{d\lambda^2} \right\rangle \right] \left(\frac{dl}{d\lambda} \right)^{-2}. \quad (3)$$

As a check of this definition, we note that the path $\Psi = \cos \theta \Phi + \sin \theta \Phi'$ considered in the introduction corresponds to $dl/d\theta = 1$ and $C|N\rangle = -|\Psi\rangle$, in other words to unit curvature and the main unit normal vector opposite to Ψ , a result which is not surprising for a meridian circle.

In the case of a path $\Psi = \exp(i\omega\lambda) \Psi_0$ where only the phase of the vector changes, this definition gives $dl/d\lambda = \omega$ and $C|N\rangle = -|\Psi\rangle$, which looks very analogous to the previous case although only one independent vector is involved. One may interpret the analogy, however, by setting $\theta = \omega\lambda$, thus

$$\Psi = \cos \theta \Psi_0 + \sin \theta (i\Psi_0),$$

and considering Ψ_0 and $i\Psi_0$ as two orthogonal Euclidian directions.

3. An illustrative example. — Let Φ_0 be any Slater determinant and $|p\rangle$ and $|h\rangle$ be, respectively, an empty and a filled orbit for Φ_0 . The corresponding fermion creation (annihilation) operators a_p^+ , a_h^+ (a_p , a_h) satisfy $a_p|\Phi_0\rangle = a_h^+|\Phi_0\rangle = 0$ and it is easy to check that the path

$$|\Phi(\lambda)\rangle = \exp[\lambda(a_p^+ a_h - a_h^+ a_p)] |\Phi_0\rangle \quad (4)$$

also can be written

$$|\Phi(\lambda)\rangle = \cos \lambda |\Phi_0\rangle + \sin \lambda |ph\rangle, \quad (5)$$

where $|ph\rangle = a_p^+ a_h |\Phi_0\rangle$ is a one-particle, one-hole state. The one-body operator $(a_p^+ a_h - a_h^+ a_p)$ in eq. (4) guarantees that $\Phi(\lambda)$ remains a Slater determinant for all values of λ . As shown by eq. (5), it turns out that this path is also a meridian circle.

Let now $|p'\rangle$ and $|h'\rangle$ be another particle and another hole states, respectively, with

$$\langle p|p'\rangle = \langle h|h'\rangle = 0.$$

It is easy to check that the new path of Slater determinants

$$|\Phi(\lambda)\rangle = \exp \{ \lambda [\theta(a_p^+ a_h - a_h^+ a_p) + \theta'(a_{p'}^+ a_{h'} - a_{h'}^+ a_{p'})] \} |\Phi_0\rangle \quad (6)$$

where θ and θ' are real, also can be written

$$|\Phi(\lambda)\rangle = \cos(\lambda\theta) \cos(\lambda\theta') |\Phi_0\rangle + \sin(\lambda\theta) \cos(\lambda\theta') |ph\rangle + \cos(\lambda\theta) \sin(\lambda\theta') |p'h'\rangle + \sin(\lambda\theta) \sin(\lambda\theta') |pp'hh'\rangle, \quad (7)$$

where $|pp'hh'\rangle = a_p^+ a_{p'}^+ a_{h'} a_h |\Phi_0\rangle$ is a two-particle, two-hole state. A straightforward calculation of the curvature at Φ_0 gives

$$C^2 = 1 + 4\theta^2\theta'^2(\theta^2 + \theta'^2)^{-2}, \quad (8)$$

which is larger than 1 in general.

It is convenient here to set the constraint

$$\theta^2 + \theta'^2 = 1,$$

Fig. 1. — Chart of the neighbourhood of a Slater determinant when only two completely distinct particle-hole pairs are available. The geodesics of weak and strong curvature are shown explicitly.

which restricts in no way the freedom of $\Phi(\lambda)$. It simplifies the search for a maximum of the curvature. One sees at once that the curvature is minimum when $\theta = 0$ or $\theta' = 0$. This corresponds to the meridian circles already met earlier. The curvature reaches a maximum, equal to $\sqrt{2}$, when $\theta = \pm \theta'$.

A chart of the neighbourhood of Φ_0 , as can be seen on figure 1, thus shows that paths along axis lines have a minimal curvature while paths along the diagonal lines have a maximal curvature. One feels intuitively that it is harder to reach a 2 particle-2 hole state than a one-particle-one-hole state.

4. Generalization. — Let Φ_0 be any Slater determinant and $\{|\alpha\rangle\}$ be a corresponding single-particle basis, with the index α running first over filled states $|h\rangle$ then empty states $|p\rangle$. Since the most general one-body, Hermitian operator A is

$$|\Phi(\lambda)\rangle = \left(1 + i\lambda \langle A \rangle - \frac{\lambda^2}{2} \langle A \rangle^2 - \frac{\lambda^2}{2} \sum_{ph} |A_{ph}|^2\right) |\Phi_0\rangle + (i\lambda - \lambda^2 \langle A \rangle) \sum_{ph} A_{ph} |ph\rangle - \lambda^2 \sum_{\substack{p < p' \\ h < h'}} (A_{ph} A_{p'h'} - A_{ph'} A_{p'h}) |pp' hh'\rangle + \dots \quad (11)$$

where

$$\langle A \rangle = \sum_h A_{hh}$$

is the expectation value of A in Φ_0 . It is seen from eq. (11) that $\langle A \rangle$ induces a phase modification of Φ_0 , which is a complication of minor interest. It will thus be assumed in the following that $\langle A \rangle = 0$.

From eqs. (3) and (11) one then finds, for $\lambda = 0$, the result

$$C|N\rangle = -|\Phi_0\rangle - 2 \sum_{\substack{p < p' \\ h < h'}} (A_{ph} A_{p'h'} - A_{ph'} A_{p'h}) |pp' hh'\rangle, \quad (12)$$

under the constraint

$$\left(\frac{dI}{d\lambda}\right)^2 = \sum_{ph} |A_{ph}|^2 = 1. \quad (13)$$

The curvature is thus given by

$$C^2 = 1 + \sum_{\substack{pp' \\ hh'}} |A_{ph} A_{p'h'} - A_{ph'} A_{p'h}|^2, \quad (14)$$

or

$$C^2 = 3 - 2 \sum_{\substack{pp' \\ hh'}} A_{ph} A_{p'h'} A_{ph'}^* A_{p'h}^*. \quad (15)$$

In the same way as in the previous section, one would like to know the directions of maximum and minimum curvature. A separability ansatz,

$$A_{ph} = B_p C_h,$$

$$A = \sum_{\alpha\beta} A_{\alpha\beta} a_\alpha^+ a_\beta, \quad (9)$$

where $A_{\alpha\beta}$ is an arbitrary Hermitian matrix, the most general path issued from Φ_0 by a straight exponential transform is

$$|\Phi(\lambda)\rangle = \exp\left(i\lambda \sum_{\alpha\beta} A_{\alpha\beta} a_\alpha^+ a_\beta\right) |\Phi_0\rangle \quad (9')$$

or

$$|\Phi(\lambda)\rangle = \left(1 + i\lambda \sum_{\alpha\beta} A_{\alpha\beta} a_\alpha^+ a_\beta - \frac{\lambda^2}{2} \sum_{\alpha\beta\alpha'\beta'} A_{\alpha\beta} A_{\alpha'\beta'} a_\alpha^+ a_\beta a_{\alpha'}^+ a_{\beta'} + \dots\right) |\Phi_0\rangle \quad (10)$$

up to second order in λ . Only that order is necessary to find the derivatives needed to calculate the curvature of the path at point Φ_0 .

A straightforward manipulation of eq. (10) gives

yields automatically a minimum $C^2 = 1$ as can be found trivially from eq. (14). In particular this occurs if $A_{ph} = 0$ for all particle-hole combinations, except for one combination $p_0 h_0$, for which $|A_{p_0 h_0}| = 1$.

To find a maximum it is useful to consider the vectors in particle space $\mathcal{A}^h$, with components

$$\mathcal{A}_p^h = A_{ph}.$$

With the scalar product

$$\mathcal{A}^h \cdot \mathcal{A}^{h'} = \sum_p A_{ph} A_{ph'}^*, \quad (16)$$

a new form of eq. (15) is found

$$C^2 = 3 - 2 \sum_{hh'} |\mathcal{A}^h \cdot \mathcal{A}^{h'}|^2. \quad (17)$$

It may be noticed that the constraint, eq. (13), reads

$$\sum_h \mathcal{A}^h \cdot \mathcal{A}^h = 1. \quad (18)$$

As a first step to maximize C^2 the numbers A_{ph} are chosen in such a way that the vectors $\mathcal{A}^h$ become orthogonal, namely $\mathcal{A}^h \cdot \mathcal{A}^{h'} = 0$ if $h \neq h'$. This is always possible since the dimension N_p of the particle space is usually larger (and even infinite) in practical calculations than the finite dimension N_h of the hole space. It is thus possible to choose N_h independent, and orthogonal, vectors $\mathcal{A}^h$ of the particle space. Then eq. (17) reduces to

$$C^2 = 3 - 2 \sum_h (\mathcal{A}^h \cdot \mathcal{A}^h)^2. \quad (19)$$

It is trivial to deduce from eq. (18) that C^2 reaches a maximum

$$C^2 = 3 - 2 \sum_h N_h^{-2} = 3 - 2 N_h^{-1}, \quad (20)$$

when all $\mathcal{A}^h \cdot \mathcal{A}^h$ are equal.

The maximum curvature is thus reached when

$$\sum_p |A_{ph}|^2 = N_h^{-1}$$

for all hole states. In other words, paths which distribute the particle-hole strength evenly between all holes (and particles) generate a larger curvature. Conversely, the curvature is minimum if the particle-hole strength $\mathcal{A}_h \cdot \mathcal{A}_h$ vanishes for all holes, except one, h_0 , with $\mathcal{A}_{h_0} \cdot \mathcal{A}_{h_0} = 1$. This result is thus a simple generalization of that expressed by the chart, figure 1.

5. Discussion and conclusion. — The physical question to be investigated is, what is the curvature of a dynamical path and whether it is influenced by the curvature properties of the manifold underlying the path. The question is not too difficult to cope with in the case of a time dependent Schrödinger path, stretching on the unit sphere. In order to get rid of the unnecessary evolution of the phase one may describe the path by the equation

$$\Psi(t) = \exp[i(E - H)t] \Psi_0, \quad (21)$$

where $E = \langle \Psi(t) | H | \Psi(t) \rangle$ is the conserved energy. One easily finds that the curvature remains a constant,

$$C^2 = \frac{\langle \Psi_0 | (H - E)^4 | \Psi_0 \rangle}{[\langle \Psi_0 | (H - E)^2 | \Psi_0 \rangle]^2} \quad (22)$$

which is obviously larger than 1 in general. If one sets $E = 0$ in eq. (22), namely if one does not compensate for the phase in eq. (21), one finds that the curvature becomes 1 for an eigenstate. This situation was already met at the end of section 2.

The curvature of a time-dependent Hartree-Fock path is more delicate to predict or analyse, for the evolution operator changes along the path. The straight exponentials considered in section 4 are thus not completely relevant. It is actually likely that the non-linear dependence of the Hartree-Fock Hamiltonian upon the Slater determinants will increase the curvature. It is also reasonable to predict that collective paths, which involve many particle-hole components, will induce systematically a large curvature as that found in section 4. The relation of paths to geodesics remains to be investigated.

The connection between large collectivity and large curvature is may be the main result to retain from this paper. It would be interesting to check in practical cases whether large collective masses would also occur in such a connection. Such an intriguing coincidence would recall other domains of physics where dynamical and geometrical features are connected and would require further investigation. It must be noticed however that the lack of isotropy which has been established in section 4 for the Slater manifold still keeps this manifold homogeneous, for the curvature properties which have been found around each determinant do not depend on that determinant. Only the Hamiltonian itself can add a dynamical structure to that manifold.

The calculation of the path curvature in the case of several well-known cases of collective motion is in progress and will be reported soon. Preliminary results on the case of traditional collective motions (translations, rotations, ...) indicate that the path curvature is indeed close to $\sqrt{3}$.

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