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Symplectic Manifolds, Coadjoint Orbits, and Mean Field Theory

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Mean field theory is given a geometrical interpretation as a Hamiltonian dynamical system. The Hartree–Fock phase space is the Grassmann manifold, a symplectic submanifold of the projective space of the full many-fermion Hilbert space. The integral curves of the Hartree–Fock vector field are the time-dependent Hartree–Fock solutions, while the critical points of the energy function are the time-independent states. The mean field theory is generalized beyond determinants to coadjoint orbit spaces of the unitary group; the Grassmann variety is the minimal coadjoint orbit.

1. INTRODUCTION

The mean field theory of atomic electrons (Hartree, 1927–28) is based upon the simple picture of a neutral atom composed of a massive, positively charged nucleus plus A orbiting electrons in states ϕ_α, $\alpha = 1, 2, \ldots, A$. The single-electron states are solutions to the Hartree equation

$$-\frac{1}{2m}\Delta\phi_\alpha - \frac{Ae^2}{r}\phi_\alpha + V_{\mathrm{H}}(\mathbf{r})\phi_\alpha = \varepsilon_\alpha\phi_\alpha \tag{1}$$

where the first term gives the kinetic energy of the electron in the state ϕ_α, the second term is its Coulomb attraction to the fixed nucleus at the origin, and the third term is its Hartree Coulomb repulsion from the orbiting electrons

$$V_{\mathrm{H}}(\mathbf{r}) = \int \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\rho(\mathbf{r}')\, d^3r' \tag{2}$$

where the density of electrons at $\mathbf{r}'$ is given by

$$\rho(\mathbf{r}') = \sum_\beta |\phi_\beta(\mathbf{r}')|^2 \tag{3}$$

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Although equation (1) has the appearance of a Hamiltonian eigenvalue problem, the Hartree potential depends upon the states through the density. Thus, it is a nonlinear equation for which the states ϕ_α must be determined self-consistently along with the Hartree mean field V_{H}.

The Hartree self-consistent equation has the advantage of being based upon a clear physical picture. On the other hand, it has the disadvantage of being wrong. The problem is that the Pauli exclusion principle has not been respected. Fock (1930) derived the correct equations using the variational principle. The only adjustment is that the local Hartree potential is replaced in equation (1) by the nonlocal Hartree–Fock mean field term

$$(V_{\mathrm{HF}}\phi_\alpha)(\mathbf{r}) = \sum_\beta \int \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\,\phi_\beta(\mathbf{r}')^*[\phi_\beta(\mathbf{r}')\phi_\alpha(\mathbf{r}) - \phi_\alpha(\mathbf{r}')\phi_\beta(\mathbf{r})]\,d^3r' \qquad (4)$$

Note that V_{HF} is the difference of two terms. The first is just the Hartree potential V_{H}, while the second is known as the exchange term.

The class of A-electron states used in the variational principle is the Slater determinants $\{\Phi = \phi_1 \wedge \phi_2 \wedge \cdots \wedge \phi_A\}$. The set of all such determinants forms a hypersurface within the vector space of all antisymmetrized wave functions (which is itself the span of the determinants).

Although Hartree–Fock theory is derived from quantum theory, the resulting mean field theory has significant structural differences from quantum mechanics. First, instead of a linear Hamiltonian eigenvalue problem, the Hartree–Fock dynamical equation is nonlinear. Second, the set of admissible states in Hartree–Fock theory does not form a vector space. The aim of this paper is to clarify the fundamental theoretical structure of mean field theories. We shall see that a mean field theory is a *classical* Hamiltonian dynamical system! The unitary group acting on the single-particle Hilbert space plays a key role in the formulation.

The analysis will make it possible to generalize Hartree–Fock theory to nondeterminantal wave functions. Also, a simple existence proof for Hartree–Fock solutions is given, using some algebraic topology. The results are not restricted to multielectron atoms and, indeed, may be applied to any finite system of interacting fermions.

2. UNITARY GROUP ORBITS

Let us suppose, for technical simplicity, that the single-particle space has finite dimension n. Then the full Hilbert space of A-fermion states is the exterior (or antisymmetrized tensor) product of A copies of the single-particle space. It has dimension $n!/[A!(n-A)!]$. The unitary group $U(n)$ acts on the single-particle space and, hence, on the A-fermion space.

The manifold of states relevant to mean field theory is the space of rays of determinants. It may be identified with the complex Grassmann variety $CG(A, n-A)$, which is the manifold of A-dimensional hyperplanes in an n-dimensional complex vector space. To see the connection, suppose that $\Phi = \phi_1 \wedge \phi_2 \wedge \cdots \wedge \phi_A$ is a ray representative. Then the hyperplane spanned by $\{\phi_1, \phi_2, \ldots, \phi_A\}$ is the corresponding point in the Grassmann variety. On the other hand, given an A-dimensional hyperplane, choose a basis $\{\phi_1, \phi_2, \ldots, \phi_A\}$ for it, thereby giving the determinant $\Phi = \phi_1 \wedge \phi_2 \wedge \cdots \wedge \phi_A$.

Hartree-Fock theory can be characterized by two properties of the $U(n)$ group action on the Grassmann variety. First, $U(n)$ acts transitively on $CG(A, n-A)$. This is proven by fixing a hyperplane and selecting an orthonormal basis $\{\psi_1, \psi_2, \ldots, \psi_A\}$ spanning it. Then, given any other hyperplane spanned by an orthonormal basis $\{\phi_1, \phi_2, \ldots, \phi_A\}$, choose $g \in U(n)$ so that $\phi_i = g\psi_i$. Thus,

$$g^{\Psi} = g\psi_1 \wedge g\psi_2 \wedge \cdots \wedge g\psi_A = \phi_1 \wedge \phi_2 \wedge \cdots \wedge \phi_A = \Phi$$

The second key property is really a consequence of the first: Elements of the Lie algebra $u(n)$ may be identified with tangent vectors to the orbit space. Let b_α^+ (respectively b_α) denote the fermion creation (respectively destruction) operator for the state ψ_α in a fixed selected orthonormal basis $\{\psi_1, \psi_2, \ldots, \psi_n\}$. For $X = (X_{\alpha\beta}) \in u(n)$, set $\hat{X} \equiv \sum_{\alpha\beta} X_{\alpha\beta} b_\alpha^+ b_\beta$. Let $\gamma_X(\tau)$ denote the curve in the direction X through Ψ lying in the space of determinants (and hence the Grassmann manifold),

$$\gamma_X(\tau) = \exp(\tau\hat{X})\Psi, \qquad -\infty < \tau < \infty \tag{5}$$

The tangent vector to this curve through Ψ may be identified with $X \in u(n)$. Since the $U(n)$ action is transitive, the tangent space at Ψ is spanned by $u(n)$. Similarly, $g\gamma_X(\tau)$ is a curve through $\Phi = g\Psi$ in the direction $Ad_g(X) = gXg^{-1}$.

Now, to derive the Hartree-Fock equation, we need only compute the critical points to the energy function $\mathcal{H}$. For Φ a normalized representative from $CG(A, n-A)$, the energy function is given by

$$\mathcal{H}(\Phi) = \langle \Phi | H\Phi \rangle \tag{6}$$

where H is the Hamiltonian operator. A critical point $\Phi = g\Psi$ of $\mathcal{H}$ is, by definition, where the derivative of the energy function vanishes in all directions tangent to the Grassmann space,

$$\begin{aligned} 0 = d\mathcal{H}(Ad_g(X)) &= \frac{d}{d\tau} \langle g\gamma_X(\tau) | Hg\gamma_X(\tau) \rangle |_{\tau=0} \\ &= \langle \Phi | [H, g\hat{X}g^{-1}]\Phi \rangle \end{aligned} \tag{7}$$

This equation is equivalent to the Hartree-Fock equation.

One advantage to this derivation of the Hartree-Fock equation is that it may be generalized to nondeterminantal wave functions. The above argument only depends upon the fact that the manifold of admissible states is an orbit of $U(n)$ in the exterior product space. Thus, if we choose any normalized A-fermion wave function Ψ and let the orbit space $\{\Phi = g\Psi | g \in U(n)\}$ be the set of admissible states, then the generalized Hartree-Fock solutions are the critical points of the energy function and therefore satisfy equation (7). Choose a single-particle basis so that $\langle\Psi|b_\rho^+ b_\sigma\Psi\rangle = \nu_\rho\delta_{\rho\sigma}$ is diagonal with occupancies ν_ρ. Then, the generalized Hartree-Fock equations for a critical point $\Phi = g\Psi$ are given by

$$\begin{aligned} 0 = (\nu_\rho - \nu_\sigma)\left[T(g)_{\rho\sigma} + \sum_\delta V(g)_{\delta\rho\delta\sigma}\nu_\delta \right] \\ + \tfrac{1}{2}[\Omega(g)_{\rho\sigma} - \Omega(g)^*_{\sigma\rho}] \end{aligned} \tag{8}$$

for a one-plus two-body Hamiltonian $H = T + V$, where

$$\begin{aligned} T(g)_{\alpha\beta} &= \sum_{\alpha'\beta'} g^{-1}_{\alpha\alpha'} T_{\alpha'\beta'} g_{\beta'\beta} \\ V(g)_{\alpha\beta\gamma\delta} &= \sum_{\alpha'\beta'\gamma'\delta'} g^{-1}_{\alpha\alpha'} g^{-1}_{\beta\beta'} V_{\alpha'\beta'\gamma'\delta'} g_{\gamma'\gamma} g_{\delta'\delta} \\ \Omega(g)_{\rho\sigma} &= \sum_{\alpha\beta\delta} V(g)_{\alpha\beta\sigma\delta}[\langle\Psi|b_\alpha^+ b_\beta^+ b_\delta b_\rho\Psi\rangle \\ &\quad - (\delta_{\alpha\rho}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\rho})\nu_\rho\nu_\delta] \end{aligned} \tag{9}$$

Note that in the case of the conventional determinantal theory, $\Omega(g) = 0$, and equation (9) reduces to the usual Hartree-Fock equations.

A significant byproduct of the analysis is a simple existence proof for Hartree-Fock solutions. First, since a $U(n)$ orbit is compact, the energy function attains its maximum and minimum on it, and there must exist at least those two solutions. But much more can be asserted in the generic case when the energy function has a nondegenerate Hessian at each critical point, i.e., there are no catastrophes. In this generic case, Morse theory can be applied, and the number of critical points of index k is at least the Betti number β_k of the $U(n)$ orbit space. For determinantal Hartree-Fock, the minimum total number of critical points is $\sum \beta_k = n!/[A!(n-A)!]$. This is a very satisfying result because this minimum number of critical points equals the dimension of the A-fermion Hilbert space and hence the number of exact eigenstates of the Hamiltonian.

3. MEAN FIELD DYNAMICS

Time-dependent Hartree-Fock theory is a natural extension of the time-independent theory. The basic dynamical equation is

$$T\phi_\alpha + V_{\mathrm{HF}}\phi_\alpha = i\,\partial\phi_\alpha/\partial t \tag{10}$$

Our aim is to discover a geometrical interpretation for this equation. Remarkably, equation (10) is a Hamiltonian dynamical equation in the sense of classical mechanics with respect to a suitably selected Poisson bracket.

Rather than define the Poisson bracket, it is both more natural and convenient to specify the equivalent symplectic form ω. This nondegenerate, antisymmetric form is defined on the determinantal orbit for pairs of tangent vectors $X,\ Y \in u(n)$ at the point Ψ by

$$\omega_\Psi(X,\ Y) = -i\langle\Psi|[\hat{X},\ \hat{Y}]\Psi\rangle \tag{11a}$$

and at the translated point $\Phi = g\Psi$ by

$$\omega_\Phi(Ad_g(X),\ Ad_g(Y)) = -i\langle\Phi|[g\hat{X}g^{-1},\ g\hat{Y}g^{-1}]\Phi\rangle \tag{11b}$$

where $Ad_g(X),\ Ad_g(Y) \in u(n)$ are tangent vectors at Φ. Note that ω is just the form inherited from the projective space of the exterior product Hilbert space

The Hartree-Fock Hamiltonian H_{HF} is the vector field tangent to the orbit satisfying the usual classical mechanics relation connecting the vector field H_{HF} with the one-form $d\mathcal{H}$ (Abraham and Marsden, 1978)

$$\omega_\Phi(H_{\mathrm{HF}}(\Phi),\ Ad_g(X)) = d\mathcal{H}(Ad_g(X)) \tag{12}$$

for every tangent vector $Ad_g(X)$ at $\Phi = g\Psi$. A time-dependent Hartree-Fock solution is an integral curve of the vector field H_{HF}. This dynamics is identical to equation (10), as may be verified by direct computation of H_{HF} in equation (12).

One would like to extend this dynamics immediately to nondeterminantal orbits. However, this is not possible, since the inherited symplectic form is only nondegenerate on the Grassmann manifold. Thus, equation (12) has no unique solution for the Hartree-Fock vector field on nondeterminantal orbits. In order to circumvent this difficulty, I consider the alternative, but equivalent, formulation of determinantal Hartree-Fock theory in terms of density matrices, which is readily generalized to nondeterminantal states.

4. COADJOINT ORBITS

The $U(n)$ group action is interrelated with the symplectic geometry on the determinantal orbit since $U(n)$ acts as a group of canonical transformations in the sense of classical mechanics,

$$\omega_\Psi(X,\ Y) = \omega_{g\Psi}(Ad_g(X),\ Ad_g(Y)) \tag{13}$$

for all $X,\ Y \in u(n)$. Hence, by the Kostant-Souriau classification theorem, the Slater determinants must be in one-to-one correspondence with (a covering space of) a coadjoint $U(n)$ orbit (Kostant, 1970; Souriau, 1970).

This equivalent version of Hartree-Fock in terms of unitary coadjoint orbits is known as the density matrix formulation (Belyaev, 1965).

A density matrix $\rho_{\alpha\beta} = i\langle\Psi|b_\beta^+ b_\alpha\Psi\rangle$ is an element of the dual space $u(n)^*$, i.e., a real-valued linear function of $u(n)$ given by

$$\rho(X) \equiv \mathrm{tr}(\rho X) = i\left\langle \Psi \middle| \sum_{\alpha\beta} X_{\alpha\beta} b_\alpha^+ b_\beta \Psi \right\rangle \tag{14}$$

The coadjoint action,

$$Ad_g^*(\rho) = g\rho g^{-1} \tag{15}$$

is compatible with the group action on the multifermion states,

$$Ad_g^*(\rho)(X) = i\left\langle g\Psi \middle| \sum_{\alpha\beta} X_{\alpha\beta} b_\alpha^+ b_\beta g\Psi \right\rangle \tag{16}$$

Lie algebra elements may be regarded as tangent vectors to coadjoint orbits, $\{Ad_g^*(\rho),\ g \in U(n)\}$, by reasoning similar to the case of wave function orbits. But, in contrast to this latter case, *every* coadjoint orbit is a symplectic manifold with the nondegenerate form

$$\omega_\rho(X, Y) = \mathrm{tr}(\rho[X, Y]) \tag{17}$$

Thus, the Hartree-Fock vector field on a coadjoint orbit is well-defined via equation (12) in terms of the energy function. A generalized time-dependent Hartree-Fock solution is an integral curve of the Hartree-Fock vector field. A time-independent Hartree-Fock solution is a point where the Hartree-Fock vector field vanishes.

5. DISCUSSION

The energy function is only unambiguously defined on the coadjoint orbit of determinantal densities. For general density orbits, the (moment) map from the A-fermion space onto the dual space $g\Psi \to g\rho g^{-1}$ is many-to-one. In order to achieve a well-defined energy function on a coadjoint orbit, an average of the Hamiltonian expectation is required (Rosensteel and Rowe, 1981).

The method reviewed here may be generalized to any Lie group acting on Fock space. The case of Hartree-Fock-Bogoliubov theory based upon the orthogonal group $O(2n)$ has been studied by Rosensteel (1981).

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REFERENCES

Abraham, R., and Marsden, J. E. (1978). *Foundations of Mechanics*, §3.3, Benjamin, Reading, Massachusetts.
Belyaev, S. (1965). *Nuclear Physics*, **64**, 17.
Fock, V. (1930) *Zeitschrift für Physik*, **61**, 126.
Hartree, D. R. (1927–28). *Proceedings of the Cambridge Philosophical Society*, **24**, 89.
Kostant, B. (1970). In *Lecture Notes in Mathematics*, Vol. 170, Springer, New York.
Rosensteel, G. (1981). *Physical Review A*, **23**, 2794.
Rosensteel, G., and Ihrig, E. (1980). *Journal of Mathematical Physics*, **21**, 2297.
Rosensteel, G., and Rowe, D. J. (1981). *Physical Review A*, **24**, 673.
Souriau, J. M. (1970). *Structure des Systemes Dynamiques*, Dunod, Paris.