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Many-body quantum mechanics as a symplectic dynamical system

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An approach is formulated to the problem of obtaining approximate solutions to many-body quantum mechanics. The starting point is the representation of quantum mechanics as Hamiltonian mechanics on a symplectic manifold (phase space). It is shown that Dirac's variation of an action integral provides a natural mechanism for constraining the dynamics to symplectic submanifolds and gives rise to a hierarchy of approximate many-body theories of which Hartree-Fock, random-phase approximation, time-dependent Hartree-Fock, and the double commutator equations of motion formalism are special cases.

I. INTRODUCTION

Two fundamental methods of obtaining approximate solutions to the many-body problem are to truncate the Hilbert space and to restrict consideration to a class of trial wave functions. An example of the former is the shell model in which one diagonalizes the Hamiltonian in a finite-dimensional shell-model space. An example of the latter is the Hartree-Fock approximation in which one minimizes the energy expectation in the space of Slater determinants. Whereas the shell-model space is itself a Hilbert space, the set of Slater determinants constitutes a hypersurface within the Hilbert space but is not itself a Hilbert space. As a consequence many significant properties of quantum mechanics on Hilbert spaces are lost, e.g., the superposition principle. However, if one is interested, for example, in large amplitude collective phenomena like fission or heavy-ion reactions which cannot reasonably be described within the confines of a small linear subspace of the Hilbert space, this is a price one may be willing to pay. Furthermore, some really good approximate theories can result and more than compensate for the losses; examples are the Hartree-Fock (HF) approximation, the random-phase approximation (RPA), time-dependent Hartree-Fock theory (TDHF), and Hartree-Bogolyubov theory.[1]

In the following section, we consider many-body quantum mechanics as a Hamiltonian mechanics on a symplectic manifold. Symplectic manifolds are fundamental in both classical and quantum mechanics because they are phase spaces; i.e., they are real even dimensional manifolds with a Poisson bracket structure as discussed in Sec. II. If $\mathcal{H}$ is the Hilbert space, the fundamental symplectic manifold of quantum mechanics is the projective space $P\mathcal{H}$ of all one-dimensional subspaces or rays of $\mathcal{H}$. Equivalently, $P\mathcal{H}$ may be defined as the space of states in $\mathcal{H}$ with unit modulus together with an equivalence relation

$$|\Psi\rangle \equiv e^{i\delta}|\Psi\rangle , \tag{1.1}$$

which identifies states differing only by a phase factor. Unlike the phase space of classical mechanics, which for N particles is of dimension $6N$, the phase space $P\mathcal{H}$ is infinite dimensional. However, in practical calculations one invariably restricts the Hilbert space to finite dimensions. To avoid some of the pitfalls associated with infinite-dimensional manifolds, we therefore assume that $P\mathcal{H}$ is of indefinitely large but, nevertheless, finite dimension.

Now it is well known that the eigenstates of the Hamiltonian are given by the points on $P\mathcal{H}$ at which the energy expectation is stationary. We shall also see that the solutions of the time-dependent Schrödinger equation trace out paths on $P\mathcal{H}$ given by Hamilton equations of motion. Furthermore, the time-dependent solutions corresponding to small amplitude normal mode vibrations about a stationary point provide detailed and precise information about the spectroscopy of the system. Thus although $P\mathcal{H}$ is not a Hilbert space, it nevertheless supports a complete and exact formulation of quantum mechanics.

When the many-body problem is formulated in this way, approximate theories are immediately obtained by simply restricting the dynamics to a symplectic submanifold of $P\mathcal{H}$. Clearly it is at this point that physical insight is needed to discover useful and realistic submanifolds. For example, experimental observations often lead one to suppose that, to a good approximation, certain collective degrees of freedom are decoupled from

the other (intrinsic) degrees of freedom. Thus one might attempt a describtion of collective states by constraining the dynamics to a corresponding collective submanifold. Of particular relevance to many-fermion theory is the constraint to the Grassman manifold of Slater determinants. Slater determinants, or simple states as we shall call them, play a central role in many-fermion theory fundamentally because we cannot solve the many-body problem and so resort to independent-particle approximations of one kind or another. It is not surprising therefore that the Grassman manifold has many simple and useful properties. However, many of its properties derive not so much from its independent-particle character as from the fact that it is a symplectic manifold. Furthermore, being an orbit of the group of one-body unitary transformations, it is also a homogeneous space. And these properties are shared with other symplectic manifolds and homogeneous spaces. When the dynamics is constrained to the Grassman manifold, the stationary states are the HF states, the normal model vibrations give the RPA and Hamilton's equations are the TDHF equations. However, there is obviously a wealth of other symplectic submanifolds to be explored each of which, as we shall show, supports it counterpart of the HF, RPA, and TDHF theories.

II. CONSTRAINED HAMILTONIAN DYNAMICS AND SYMPLECTIC GEOMETRY

A. Classical dynamics

A classical phase space M is a smooth manifold with a Poisson bracket structure. If $C^\infty(\mathrm{M})$ denotes the smooth real-valued functions on M, the Poisson bracket $\{\ ,\ \}$ is an antisymmetric bilinear product on $C^\infty(\mathrm{M})$ that satisfies the Jacobi identity; i.e.,

$$\{F,G\}+\{G,F\}=0\,, \tag{2.1}$$

$$\{\{F,G\},K\}+\{\{G,K\},F\}+\{\{K,F\},G\}=0\,, \tag{2.2}$$

for any F, G, and $K\in C^\infty(\mathrm{M})$. Thus $C^\infty(\mathrm{M})$ is a Lie algebra with the Poisson bracket for Lie product. A classical phase space is also required to admit canonical coordinate charts. Canonical coordinates, conventionally denoted $(p_1, p_2, \ldots, q^1, q^2, \ldots,)$, are required to satisfy the familiar relations

$$\begin{aligned}&\{q^\alpha,q^\beta\}=\{p_\alpha,p_\beta\}=0\,,\\ &\{p_\alpha,q^\beta\}=\delta^\beta_\alpha\,.\end{aligned} \tag{2.3}$$

Thus an arbitrary coordinate chart $(x^1,x^2,\ldots,)$ for a neighborhood of M is said to be *locally canonical* if the matrix

$$\sigma^{\mu\nu}=\{x^\nu,x^\mu\} \tag{2.4}$$

is of the canonical form

$$(\sigma^{\mu\nu})=\begin{pmatrix}0 & -I\\ I & 0\end{pmatrix} \tag{2.5}$$

at each point of the neighborhood, where I is the unit matrix. Clearly a necessary (and in fact, by Darboux's theorem,[2] sufficient) condition for the existence of local canonical coordinate charts is that the matrix $(\sigma^{\mu\nu})$, defined by Eq. (2.4), is invertable. A Hamiltonian dynamics on M is now defined by introducing the Hamiltonian (energy) function H and the equation of motion

$$\dot F=\{H,F\} \tag{2.6}$$

for any $F\in C^\infty(\mathrm{M})$, where $\dot F=dF/dt$.

The above properties of a classical phase space are precisely those of a symplectic manifold. The relationship between the Poisson bracket and symplectic structures has been discussed by several authors[2-4] and is exhibited explicitly in the following subsection. Indeed symplectic manifolds are the natural settings for Hamiltonian dynamics. Furthermore, Hamiltonian subdynamics are naturally obtained by restricting the dynamics to symplectic submanifolds. Again an explicit demonstration of how this is done is given in the quantal context in the following subsection.

B. Quantum dynamics

A Hilbert space $\mathcal{H}$ is a complex linear space with a Hermitian inner product $\langle\Psi|\Phi\rangle$. In order to regard it as a phase space, we treat it as a real linear space of couble the dimension, i.e., each basis state $|\psi_\nu\rangle$ is replaced by the pair $|\psi_\nu\rangle$ and $i|\psi_\nu\rangle$. There are now two natural real nondegenerate forms on this realified Hilbert space, namely, $\mathrm{Re}\langle\Psi|\Phi\rangle$ and $\mathrm{Im}\langle\Psi|\Phi\rangle$. The former being symmetric and positive-definite is Riemannian and enables one to introduce concepts of distance, angle, and curvature, etc. The latter being antisymmetric and closed is symplectic and is what makes $\mathcal{H}$ and its associated projective space $P\mathcal{H}$ phase spaces.

Suppose that M is a submanifold of either $\mathcal{H}$ or $P\mathcal{H}$ and

$$H(\Psi)=\langle\Psi|\mathrm{H}|\Psi\rangle \tag{2.7}$$

is the energy function on M, where H is the Hamiltonian. The starting point for Dirac's formulation[5] of constrained quantal dynamics is the extremal condition of an action integral

$$\delta\int_{t_1}^{t_2}\left\langle\Psi(t)\left|i\frac{\partial}{\partial t}-\mathrm{H}\right|\Psi(t)\right\rangle dt=0\,, \tag{2.8}$$

which yields the differential equation

$$dH=i(\langle d\Psi|\dot\Psi\rangle-\langle\dot\Psi|d\Psi\rangle)\,, \tag{2.9}$$

where $\dot{\Psi} = \partial\Psi/\partial t$. In terms of coordinates $(x^1, x^2, \ldots,)$ for a neighborhood of M, this equation becomes

$$\frac{\partial H}{\partial x^\mu} = -2\,\mathrm{Im}\left\langle \frac{\partial\Psi}{\partial x^\mu} \middle| \dot{\Psi} \right\rangle = \sigma_{\mu\nu}\dot{x}^\nu, \tag{2.10}$$

where σ is the symplectic metric with components

$$\sigma_{\mu\nu} = -2\,\mathrm{Im}\left\langle \frac{\partial\Psi}{\partial x^\mu} \middle| \frac{\partial\Psi}{\partial x^\nu} \right\rangle . \tag{2.11}$$

If this metric is nondegenerate, the matrix $(\sigma_{\mu\nu})$ can be inverted to give Hamilton's equation of motion

$$\dot{x}^\mu = \sigma^{\mu\nu}\partial H/\partial x^\nu . \tag{2.12}$$

On the other hand, if σ is degenerate, Eq. (2.10) and hence (2.8) do not define an equation of motion.

Observe that we have deliberately avoided specifying a choice of coordinates in order to exhibit the coordinate independence of the equations. One way to introduce coordinates, for example, is by means of a set of observables (X^ν) whose expectation values $x^\nu = \langle\psi|X^\nu|\psi\rangle$ serve to uniquely distinguish states in some neighborhood of M (the domain of the coordinate chart). The coordinate derivatives $\partial\psi/\partial x^\nu$ are then well defined at each point in the neighborhood and are observed to be tangent to M. Convenient ways to construct coordinates in the especially interesting case when M is a homogeneous space are given in Sec. IV.

In terms of local canonical coordinates, Hamilton's equations (2.12) assume the familiar canonical form

$$\dot{p}_\alpha = -\partial H/\partial q^\alpha, \quad \dot{q}^\alpha = \partial H/\partial p_\alpha . \tag{2.13}$$

For example, if $\mathrm{M} = \mathcal{H}$ and (ψ_ν) is a basis for $\mathcal{H}$, canonical coordinates are given by the expansion

$$\psi = (1/\sqrt{2})\sum_\nu (q^\nu + ip_\nu)\psi_\nu .$$

The Poisson bracket of any two smooth functions F and G on M can now be defined in the standard way by

$$\{F, G\} = \sigma^{\mu\nu}\frac{\partial F}{\partial x^\nu}\frac{\partial G}{\partial x^\mu} . \tag{2.14}$$

However, before accepting this definition of the Poisson bracket, one must ascertain that it satisfies the requirements (2.1) and (2.2). Evidently it is bilinear and from the definition (2.11) of σ antisymmetric. Furthermore, it follows directly from Eq. (2.14) that

$$\{\{F, G\}, K\} + \{\{G, K\}, F\} + \{\{K, F\}, G\} = F^\kappa G^\lambda K^\nu(\partial\sigma_{\lambda\nu}/\partial x^\kappa + \partial\sigma_{\nu\kappa}/\partial x^\lambda + \partial\sigma_{\kappa\lambda}/\partial x^\nu), \tag{2.15}$$

where $F^\lambda = \sigma^{\lambda\kappa}\partial F/\partial x^\kappa$. With the symplectic metric defined by Eq. (2.11), one readily ascertains that

$$\partial\sigma_{\lambda\nu}/\partial x^\kappa + \partial\sigma_{\nu\kappa}/\partial x^\lambda + \partial\sigma_{\kappa\lambda}/\partial x^\nu = 0 \tag{2.16}$$

in any coordinate chart. Thus we obtain the Jacobi identity. Finally, from Eqs. (2.12) and (2.14), we obtain the equation of motion

$$\dot{F} = \{H, F\} . \tag{2.17}$$

Equation (2.16) is an expression of the fact that the symplectic metric σ, defined by Eq. (2.11), is closed (i.e., $d\sigma = 0$) on any submanifold of the Hilbert space. (One can see that this is so immediately by observing that $\sigma = d\omega$ where ω is the one form $\omega = \mathrm{Im}\langle d\Psi|\Psi\rangle$.) If, in addition, σ is nondegenerate we say that the submanifold M is symplectic. Now we have seen above that Eq. (2.8) does not define an equation of motion when σ is degenerate. Thus we conclude that *the action integral of Eq. (2.8) does not have extremal paths on a nonsymplectic submanifold.*

For example, the variational Eq. (2.8) does not define extremal paths on the manifold of Slater determinants of unit modulus. This manifold is of odd dimension and therefore cannot be symplectic. To make it symplectic one must either project onto a smaller manifold by identifying states which differ only in phase [cf. Eq. (1.1)] or add back the extra dimension by including determinants of nonunit norm as Lichtner *et al.*[6] have observed. The virtue of the latter option is that one gains the possibility of determining the time evolution of the phase. Since the phase is usually of no interest and since the Hamiltonian is norm conserving it is customary to suppress the phase and consider only symplectic submanifolds of the projective space $P\mathcal{H}$.

Another example of special interest is when $\mathrm{M} = P\mathcal{H}$. Consider real functions F and G on $P\mathcal{H}$ expressable as expectations of some Hermitian quantal observables F and G; i.e.,

$$F(\Psi) = \langle\Psi|\mathrm{F}|\Psi\rangle . \tag{2.18}$$

It can be shown that

$$\{F, G\}(\Psi) = i\langle\Psi|[\mathrm{F}, \mathrm{G}]|\Psi\rangle = -2\,\mathrm{Im}\langle\mathrm{F}\Psi|\mathrm{G}\Psi\rangle , \tag{2.19}$$

which directly relates in a coordinate-free way, the Poisson bracket and symplectic structures on $P\mathcal{H}$. Thus the equation of motion (2.17) for a function on $P\mathcal{H}$ becomes

$$\dot{F} = i\langle\Psi|[\mathrm{H}, \mathrm{F}]|\Psi\rangle \tag{2.20}$$

and the formulation of quantum mechanics as a Hamiltonian dynamics on $P\mathcal{H}$ is seen to be essentially the content of Ehrenfest's theorem.[7] How-

ever, it must be emphasized that we are primarily interested here in constrained quantal dynamics and that Eqs. (2.19) and (2.20) are not generally valid on a symplectic submanifold of $P\mathcal{H}$. It is important therefore to consider carefully in what manner the dynamics is most appropriately constrained.

We claim that Dirac's formulation is natural for the following reason. Suppose that an unconstrained trajectory in $P\mathcal{H}$ lies in $M \subset P\mathcal{H}$. If the constraining procedure is natural then we expect this trajectory to also be a solution for the constrained problem. It is clear that Dirac's procedure possesses this property since an unconstrained trajectory makes the action stationary against all variations that lie in M.

III. STATIONARY STATES AND NORMAL MODES

If H is the Hamiltonian function on a symplectic submanifold M of the projective Hilbert space $P\mathcal{H}$, we can define the energy gradiant dH as the covector field with components $(\partial H/\partial x^\nu)$, with respect to any coordinate chart (x^ν). It follows therefore, from the equation of motion (2.12) that the stationary points on M are the points at which

$$dH = 0 . \tag{3.1}$$

When M is the Grassman manifold, this equation is the Hartree-Fock equation and its solutions can be obtained by the Hartree self-consistent-field method, when it converges.[8] More generally, it can be solved[9] by the Newton-Kantorovic method,[10] which will be discussed in detail in a subsequent paper.[11]

A normal-mode solution of Hamilton's equation on M is by definition a small amplitude periodic oscillation about a stationary point. Thus, if F is any function on M, the value $F(t)$ of F at the oscillating point must be of the form

$$F(t) = F_0 + F_1 e^{-i\omega t} + F_1^* e^{i\omega t} . \tag{3.2}$$

To find the normal-mode solutions, consider a coordinate chart (x^ν) with a stationary point as origin. We may then expand the Hamiltonian function

$$H(x) = H(0) + \tfrac{1}{2} x^\mu x^\nu \frac{\partial^2 H}{\partial x^\mu \partial x^\nu} + \cdots . \tag{3.3}$$

Now, by a linear transformation, we can bring the symplectic metric to canonical form [cf. Eq. (2.5)], at the stationary point and then by a further linear canonical transformation, diagonalize the Hessian matrix $(\partial^2 H/\partial x^\mu \partial x^\nu)$. By so doing, we obtain $H(x)$ in the canonical form

$$H(x) = H(0) + \tfrac{1}{2} \sum_\alpha [B^\alpha (p_\alpha)^2 + C_\alpha (q^\alpha)^2] + \cdots . \tag{3.4}$$

It is known by a theorem of Thouless[12] that this can always be done when the stationary point is an energy minimum. The general circumstances under which the Hessian takes this canonical form have been discussed by Williamson.[13] Although the values of the coefficients B^α and C_α depend on the chart, the products $C_\alpha B^\alpha$ (no summation) and the number of positive and negative coefficients do not.[14] Thus, the equations of motion (2.13) give (there is no summation in either equation)

$$\begin{aligned} q^\alpha &= B^\alpha p_\alpha + O(x^2) , \\ \dot{p}_\alpha &= -C_\alpha q^\alpha + O(x^2) , \end{aligned} \tag{3.5}$$

which have the periodic oscillatory solutions

$$\begin{aligned} q^\alpha(t) &= \epsilon_\alpha \cos\omega_\alpha t + O(x^2) , \\ p_\alpha(t) &= -\epsilon_\alpha \omega_\alpha B_\alpha \sin\omega_\alpha t + O(x^2) , \end{aligned} \tag{3.6}$$

where $B_\alpha = (B^\alpha)^{-1}$ and $\omega_\alpha^2 = C_\alpha B^\alpha$. Writing

$$F(t) = F_0 + \frac{\partial F}{\partial q^\alpha} q^\alpha(t) + \frac{\partial F}{\partial p_\alpha} p_\alpha(t) \tag{3.7}$$

and putting $\epsilon_\alpha = \delta_{\lambda\alpha}\epsilon$ we obtain the desired result

$$F(t) = F_0 + \tfrac{1}{2}\epsilon \left[\left(\frac{\partial F}{\partial q^\lambda} + i\omega_\lambda B_\lambda \frac{\partial F}{\partial p_\lambda} \right) e^{i\omega_\lambda t} + \text{c.c.} \right] . \tag{3.8}$$

Consider now the interpretation of the above results. Equation (3.1) is the familiar variational equation for approximate eigenstates of the Hamiltonian. This variational principle is known to be good for the ground-state energy. It is then an energy minimization principle and gives an upper bound for the ground-state energy.

At the energy minimum the Hessian is clearly positive semidefinite having zero eigenvalues only if the minimum is not a single point but rather a higher-dimensional subset of points. Such situations are well known and occur, for example, whenever the variational ground state has less symmetry than the Hamiltonian, e.g., it is not rotationally invariant. We conclude then that, at the variational ground state, the parameters B^α and C_α are nonnegative and hence that the normal-mode frequencies ω_α are all real in accord with the obvious generalization of Thouless's theorem[12] for RPA frequencies. Conversely, if the normal-mode frequencies are not real, we may conclude that the stationary state is not an energy minimum.[14]

Now if $M = P\mathcal{H}$ and $|\psi_0\rangle \in M$ is the true ground state, normal-mode oscillations about $|\psi_0\rangle$ are given to first order in a small amplitude parameter δ by the states

$$|\Psi(t)\rangle \equiv |\psi_0\rangle e^{-iE_0 t} + \delta |\psi_\lambda\rangle e^{-iE_\lambda t} , \tag{3.9}$$

where $|\psi_\lambda\rangle$ is an excited eigenstate. Furthermore, if F is any observable, its expectation $F(t)$

$= \langle \Psi(t) | F | \Psi(t) \rangle$ is given by

$$F(t) = F_0 + \delta(F_{\lambda 0} e^{i(E_\lambda - E_0)t} + \text{c.c.}), \tag{3.10}$$

where

$$F_{\lambda 0} = \langle \psi_\lambda | F | \psi_0 \rangle . \tag{3.11}$$

Thus comparing this equation with Eq. (3.8) we interpret the normal-mode frequencies as the excitation energies

$$\omega_\lambda = E_\lambda - E_0 \tag{3.12}$$

and we obtain the matrix elements

$$\langle \psi_\lambda | F | \psi_0 \rangle = \frac{1}{2} \frac{\epsilon}{\delta} \left(\frac{\partial F}{\partial q^\lambda} + i\omega_\lambda B_\lambda \frac{\partial F}{\partial p_\lambda} \right) . \tag{3.13}$$

The ratio ϵ/δ is evaluated by comparing the vibrational energy $\Delta E = \delta^2 \omega_\lambda$, obtained from Eq. (3.9), with the expression $\Delta E = \frac{1}{2} \omega_\lambda^2 B_\lambda \epsilon^2$ obtained from Eqs. (3.4)–(3.6). We obtain $\epsilon/\delta = (2/\omega_\lambda B_\lambda)^{1/2}$ and hence the matrix elements

$$\langle \psi_\lambda | F | \psi_0 \rangle = (2\omega_\lambda B_\lambda)^{-1/2} \left(\frac{\partial F}{\partial q^\lambda} + i\omega_\lambda B_\lambda \frac{\partial F}{\partial p_\lambda} \right) . \tag{3.14}$$

Equations (3.12) and (3.14) which are seen to be exact on $P\mathcal{H}$, provide useful approximate theories of excited states associated with suitably chosen symplectic submanifolds of $P\mathcal{H}$. In particular, when M is the Grassman manifold these equations are the RPA equations. More generally, they are a geometrical formulation of the double commutator equations-of-motion theory of excited states.[15]

It is of interest to note that whereas the tangent space to a submanifold of the Hilbert space at a critical point is a linear subspace of the Hilbert space, the above theory of excitations does not correspond simply to the Schrödinger dynamics obtained by restricting the Hamiltonian to this linear subspace. The latter might be called a generalized Tamm-Dancoff approach.[1] In contrast, the above approach based on the normal-mode oscillations of the constrained Hamiltonian dynamics corresponds to a generalized random-phase approximation[1] which is known to be superior in many respects.

IV. HOMOGENEOUS SPACES

Consider a Lie group G acting on the Hilbert space $\mathcal{H}$. If $|\Psi(0)\rangle$ is any state in $\mathcal{H}$, the orbit of G in $\mathcal{H}$ containing $|\Psi(0)\rangle$ is the set of states

$$\mathrm{M} = \{ |\Psi(g)\rangle = g|\Psi(0)\rangle \, ; g \in \mathrm{G} \} . \tag{4.1}$$

In general, a given group has many orbits for different choices of $|\psi(0)\rangle$. Orbits of Lie groups constitute an important class of manifolds called homogeneous spaces. We anticipate that they will prove to be extremely useful in the extraction of collective subdynamics from the many-body dynamics when one is given a group of collective transformations. They are also simple to work with because their properties can be inferred from the properties of the associated groups and their isotropy subgroups.

If $|\Psi(0)\rangle \in \mathrm{M}$, as defined above, the isotropy subgroup (the little group) L at $|\Psi(0)\rangle$ is defined as the set of all elements $l \in \mathrm{G}$ that leave $|\Psi(0)\rangle$ invariant up to whatever equivalence relationships one may choose to introduce, i.e.,

$$l\,|\Psi(0)\rangle \equiv |\Psi(0)\rangle, \quad l \in \mathrm{L} \subset \mathrm{G} . \tag{4.2}$$

We can therefore write

$$|\Psi(g)\rangle \equiv |\Psi(g\mathrm{L})\rangle \equiv g\mathrm{L}\,|\Psi(0)\rangle , \tag{4.3}$$

where gL is the coset in G/L containing $g \in$ G. This expression defines a well-known diffeomorphism between M and G/L and, in particular, induces coordinate charts on M from the natural charts on G/L.

Let $\tilde{g}$ and $\tilde{l}$ denote, respectively, the Lie algebras of G and L and let $\tilde{k}$ denote a vector space complement of $\tilde{l}$ in $\tilde{g}$; i.e.,

$$\tilde{g} = \tilde{l} \oplus \tilde{k} . \tag{4.4}$$

Now it is well known that any element gL in some neighborhood of the identity in G/L can be expressed as the exponential $g\mathrm{L} = \exp(X)\mathrm{L}$ of a vector $X \in \tilde{k}$. Thus if (X_ν) is a basis for $\tilde{k}$, a coordinate chart (x^ν) for a neighborhood of $|\psi_0\rangle \in \mathrm{M}$ is defined by

$$|\Psi(x)\rangle \equiv \exp[x^\nu X_\nu]\,|\Psi(0)\rangle . \tag{4.5}$$

If the action of G on $\mathcal{H}$ is unitary then, by introducing the equivalence relation (1.1), the orbit M containing $|\Psi(0)\rangle \in P\mathcal{H}$ is a submanifold of $P\mathcal{H}$. Furthermore the operators (X_ν) are skew-Hermitian. However, M may or may not be symplectic. For the remainder of this section we shall assume that G is unitary and that $\mathrm{M} \subset P\mathcal{H}$.

Applying the general expressions of Sec. III to the homogeneous space M, we see that the energy function H on M is stationary at $|\Psi(0)\rangle$, if and only if,

$$\left(\frac{\partial H}{\partial x^\nu} \right)_{x=0} = \langle \Psi(0) | [H, \mathrm{X}_\nu] | \Psi(0) \rangle = 0 , \quad \text{all } \nu . \tag{4.6}$$

This is the familiar Rayleigh-Ritz form of the variational principle.[7]

The symplectic metric, Eq. (2.11), is given at $|\Psi(0)\rangle$ by

$$\sigma_{\mu\nu} = -i \langle \Psi(0) | [\mathrm{X}_\mu, \mathrm{X}_\nu] | \Psi(0) \rangle \tag{4.7}$$

and the Hessian by

$$\frac{\partial^2 H}{\partial x^\mu \partial x^\nu} = -\langle \Psi(0) | [X_\mu, [H, X_\nu]] | \Psi(0) \rangle . \tag{4.8}$$

Thus bringing the coordinates and the Hessian into canonical form at $|\psi(0)\rangle$ means finding a basis $(X_\nu) = (iQ^\alpha, -iP_\alpha)$ for $\tilde{k}$ such that

$$\begin{aligned}
&\langle \Psi(0) | [Q^\alpha, Q^\beta] | \Psi(0) \rangle = \langle \Psi(0) | [P_\alpha, P_\beta] | \Psi(0) \rangle = 0 , \\
&\langle \Psi(0) | [Q^\alpha, P_\beta] | \Psi(0) \rangle = i\delta^\alpha_\beta , \qquad (4.9) \\
&\langle \Phi(0) | [Q^\alpha, \mathrm{H}, P_\beta] | \Psi(0) \rangle = 0 , \\
&\langle \Psi(0) | [Q^\alpha, \mathrm{H}, Q^\beta] | \Psi(0) \rangle = \delta_{\alpha\beta} B^\alpha , \\
&\langle \Psi(0) | [P_\alpha, \mathrm{H}, P_\beta] | \Psi(0) \rangle = \delta_{\alpha\beta} C_\alpha , \qquad (4.10)
\end{aligned}$$

where the double commutator is defined

$$2[A, \mathrm{H}, B] = [A, [\mathrm{H}, B]] + [[A, H], B] . \tag{4.11}$$

It is clear that the above equations only have solutions when the metric is nondegenerate, i.e., when M is symplectic. Finally, one obtains the transition matrix elements from Eq. (3.14),

$$\langle \Psi_\lambda | \mathrm{F} | \Psi_0 \rangle = \langle \Psi(0) | [\mathrm{O}_\lambda, \mathrm{F}] | \Psi(0) \rangle , \tag{4.12}$$

where

$$\mathrm{O}_\lambda = -(\omega_\lambda B_\lambda / 2)^{1/2} \left(Q_\lambda + \frac{i}{\omega_\lambda B_\lambda} P_\lambda \right) . \tag{4.13}$$

As a practical matter, it is usually simpler to attempt a solution to Eqs. (4.9)–(4.11) by writing them in terms of the operators (O_λ) defined by Eq. (4.13) and their Hermitian adjoints $(\mathrm{O}^\dagger_\lambda)$. The equations then become

$$\begin{aligned}
&\langle \Psi_0 | [\mathrm{O}_\kappa, \mathrm{H}, \mathrm{O}^\dagger_\lambda] | \Psi_0 \rangle = \omega_\lambda \langle \Psi_0 | [\mathrm{O}_\kappa, \mathrm{O}^\dagger_\lambda] | \Psi_0 \rangle = \delta_{\kappa\lambda} \omega_\lambda , \\
&\langle \Psi_0 | [\mathrm{O}^\dagger_\kappa, \mathrm{H}, \mathrm{O}^\dagger_\lambda] | \Psi_0 \rangle = \omega_\lambda \langle \Psi_0 | [\mathrm{O}^\dagger_\kappa, \mathrm{O}^\dagger_\lambda] | \Psi_0 \rangle = 0 , \\
&\langle \Psi_0 | [\mathrm{O}_\kappa, \mathrm{H}, \mathrm{O}_\lambda] | \Psi_0 \rangle = -\omega_\lambda \langle \Psi_0 | [\mathrm{O}_\kappa, \mathrm{O}_\lambda] | \Psi_0 \rangle = 0 ,
\end{aligned} \tag{4.14}$$

which are now clearly recognizable as the fundamental equations of the double commutator equations of motion formalism.[15] Thus we confirm that the geometrical formulation of these equations given in Sec. III is a generalization of the equations-of-motion formalism to an arbitrary symplectic manifold.

V. THE GRASSMAN MANIFOLD Gr_N

An N-particle Slater determinant is the exterior (i.e., fully antisymmetrized) product of N single-particle states, i.e.,

$$\Psi_{\alpha\beta\gamma\ldots} = \psi_{\alpha\mathbf{A}} \psi_{\beta\mathbf{A}} \psi_{\gamma\mathbf{A}} \cdots . \tag{5.1}$$

Such states are called *simple*. The set of all simple states of unit modulus together with the equivalence relation (1.1), which identifies states differing only in phase, constitutes a manifold known in the mathematical literature as the Grassman manifold and denoted Gr_N. We review here some of its properties of relevance to the many-fermion problem.

Let $U(\mathcal{H}^{(1)})$ denote the group of unitary transformations of the single-particle Hilbert space $\mathcal{H}^{(1)}$. If $\{\psi_\nu; \nu = 1, 2, \ldots,\}$ is a basis for $\mathcal{H}^{1)}$, the fundamental representation of $U(\mathcal{H}^{(1)})$ is expressed

$$\psi_\nu(g) = \sum_\mu g_{\mu\nu} \psi_\mu , \quad g \in U(\mathcal{H}^{(1)}) . \tag{5.2}$$

The natural action of $U(\mathcal{H}^{(1)})$ on the N-fermion Hilbert space is then defined by the action on a basis of simple states

$$P(g)\Psi_{\alpha\beta\ldots} = \psi_\alpha(g)\psi_\beta(g)\cdots = \Psi_{\alpha\beta\ldots}(g) , \quad g \in U(\mathcal{H}^{(1)}) . \tag{5.3}$$

P is evidently the fully antisymmetric Kronecker product representation which is known to be irreducible. Now observe that this action preserves the simple character of simple states. Furthermore, since any set of N-orthonormal single-particle states uniquely defines a simple state, up to phase equivalence, and since any set of N-orthonormal single-particle states can be generated from any other such set by a unitary transformation, it follows that Gr_N is an orbit of the group $U(\mathcal{H}^{(1)})$. Thus Gr_N is a homogeneous space.

To discover the isotropy subgroup, observe that any simple state $\Psi \in \mathrm{Gr}_N$ defines a decomposition of the single-particle Hilbert space into sub-Hilbert spaces of occupied and unoccupied single-particle states, viz.,

$$\mathcal{H}^{(1)} = \mathcal{H}^{(1)}_{\mathrm{occ}} \oplus \mathcal{H}^{(1)}_{\mathrm{unocc}} .$$

Furthermore, such a decomposition in turn uniquely defines Ψ up to phase equivalence. The isotropy subgroup at $\Psi \in \mathrm{Gr}_N$ is therefore the direct product of the groups of separate unitary transformations in $\mathcal{H}^{(1)}_{\mathrm{occ}}$ and $\mathcal{H}^{(1)}_{\mathrm{unocc}}$, i.e., $U(\mathcal{H}^{(1)}_{\mathrm{occ}}) \times U(\mathcal{H}^{(1)}_{\mathrm{unocc}})$. Thus Gr_N is identified as the homogeneous space

$$\mathrm{Gr}_N \sim U(\mathcal{H}^{(1)}) / [U(\mathcal{H}^{(1)}_{\mathrm{occ}}) \times U(\mathcal{H}^{(1)}_{\mathrm{unocc}})] . \tag{5.4}$$

To define coordinate charts on Gr_N, it will be convenient to realize the Lie Algebras of the above unitary groups in the framework of second quantization. Let $\{a^\dagger_\nu; \nu = 1, 2, \ldots,\}$ and $\{a_\nu; \nu = 1, 2, \ldots,\}$ denote, respectively, a basis of single-particle creation and annihilation operators satisfying the familiar anticommutation relations

$$\begin{aligned}
&[a^\dagger_\mu, a^\dagger_\nu]_+ = [a_\mu, a_\nu]_+ = 0 , \\
&[a_\mu, a^\dagger_\nu]_+ = \delta_{\mu\nu} .
\end{aligned} \tag{5.5}$$

The Lie algebra $u(\mathcal{H}^{(1)})$ of $U(\mathcal{H}^{(1)})$ is then realized on the many-fermion Hilbert space as the set of

skew-adjoint operators

$$X = P(X^{(1)}) = \sum_{\mu\nu} X^{(1)}_{\mu\nu} a^\dagger_\mu a_\nu, \quad X^{(1)} \in u(\mathcal{H}^{(1)}) . \quad (5.6)$$

One readily ascertains that

$$[X, Y] = P([X^{(1)}, Y^{(1)}]) , \quad (5.7)$$

confirming that P is a Lie algebra homomorphism and, furthermore, that it is consistent with the group representation defined above. Thus, when we represent a simple state

$$|\alpha\beta\cdots\rangle = a^\dagger_\alpha a^\dagger_\beta \cdots |-\rangle , \quad (5.8)$$

where $|-\rangle$ is the zero-particle vacuum state, we find

$$g|\alpha\beta\cdots\rangle = a^\dagger_\alpha(g) a^\dagger_\beta(g) \cdots |-\rangle , \quad (5.9)$$

with

$$a^\dagger(g) = g a^\dagger g^{-1}, \quad g = P(g^{(1)}) \in P(U(\mathcal{H}^{(1)})) . \quad (5.10)$$

Putting $g = \exp(X)$, $X \in P(u(\mathcal{H}^{(1)}))$, we obtain

$$a^\dagger_\nu(g) = e^X a^\dagger_\nu e^{-X} = \sum_\mu g^{(1)}_{\mu\nu} a^\dagger_\mu \quad (5.11)$$

consistent with Eq. (5.2).

Now let $\{a^\dagger_h; h = 1, \ldots, N\}$ be creation operators for an orthonormal basis of single-particle states for the occupied single-particle space $\mathcal{H}^{(1)}_{occ}$ corresponding to some state $|\Psi_0\rangle \in Gr_N$. And let $\{a^\dagger_p; p = N+1, \ldots,\}$ be a similar basis for $\mathcal{H}^{(1)}_{unocc}$. We shall refer to these as hole and particle operators, respectively, in accord with standard terminology. The Lie algebra $u(\mathcal{H}^{(1)}_{occ})$ is now seen to be realized as the subset of skew-adjoint hole-hole operators

$$P(u(\mathcal{H}^{(1)}_{occ})) = \left\{ X = \sum_{h,h'=1}^{N} X_{hh'} a^\dagger_h a_{h'} ; \; X = -X^\dagger \right\} . \quad (5.12)$$

Similarly $u(\mathcal{H}^{(1)}_{unocc})$ is realized as the subset of skew-adjoint particle-particle operators

$$P(u(\mathcal{H}^{(1)}_{unocc})) = \left\{ X = \sum_{p,p'>N} X_{pp'} a^\dagger_p a_{p'} ; \; X = X^\dagger \right\} . \quad (5.13)$$

An obvious candidate for $\tilde{k}$, a vector space complement of $P[u(\mathcal{H}^{(1)}_{occ}) \oplus u(\mathcal{H}^{(1)}_{unocc})]$ in $P(u(\mathcal{H}^{(1)}))$, is therefore the subset of skew-adjoint particle-hole operators

$$\tilde{k} = \left\{ X = \sum_{p>N} \sum_{h=1}^{N} (X_{ph} a^\dagger_p a_h - X^*_{ph} a^\dagger_h a_p) \right\} \quad (5.14)$$

where the asterisk denotes complex conjugation. Finally, a basis for $\tilde{k}$ induces a coordinate chart for Gr_N in a neighborhood of the "particle-hole vacuum state" $|\Psi_0\rangle$, by means of Eq. (4.5). For example, the basis $(X_\nu) = (iQ^{ph}, -iP_{ph})$ where

$$Q^{ph} = \frac{1}{\sqrt{2}} (a^\dagger_p a_h + a^\dagger_h a_p) ,$$
$$P_{ph} = \frac{i}{\sqrt{2}} (a^\dagger_p a_h - a^\dagger_h a_p) , \quad (5.15)$$

defines the coordinate chart (p_{ph}, q^{ph}) about Ψ_0 by

$$|\Psi(p,q)\rangle = \exp i \sum_{ph} (p_{ph} Q^{ph} - q^{ph} P_{ph}) |\Psi_0\rangle . \quad (5.16)$$

This chart is seen to be canonical at $|\Psi_0\rangle$ [cf. Eq. (4.9)] since

$$\langle\Psi_0|[Q^{ph}, Q^{p'h'}]|\Psi_0\rangle = \langle\Psi_0|[P_{ph}, P_{p'h'}]|\Psi_0\rangle = 0 ,$$
$$\langle\Psi_0|[Q^{ph}, P_{p'h'}]|\Psi_0\rangle = i\delta^p_{p'} \delta^h_{h'} . \quad (5.17)$$

It should be emphasized that the above choice of $\tilde{k}$, although natural, is by no means unique. It is natural because, as one can easily show, $\tilde{k}$ is then the orthogonal complement of the isotropy subalgebra with respect to the Riemannian metric induced from the real part of the Hilbert-space inner product, i.e., the real counterpart of the symplectic metric (2.5). This Riemannian structure is identical to the Killing form on $u(\mathcal{H}^1)$. This came about because we defined $\tilde{k}$ in terms of an orthonormal basis of single-particle states. This choice is also convenient for the construction of coordinate charts for Gr_N in view of the following useful theorem:

Theorem. If Ψ_0 is any normalized simple N-particle state and $(a^\dagger_h; h = 1, \ldots, N)$ and $(a_p; p = N+1, \ldots,)$ are, respectively, single-particle creation operators for an orthonormal basis of hole and particle states defined with respect to Ψ_0 as particle-hole vacuum, then any other normalized simple N-particle state Ψ can be expressed, to within a phase factor, by

$$|\Psi\rangle \equiv \exp \sum_{ph} (X_{ph} a^\dagger_p a_h - X^*_{ph} a^\dagger_h a_p) |\Psi_0\rangle , \quad (5.18)$$

where (X_{ph}) is a set of complex numbers.

The proof of this theorem is given in the appendix. Note that it is distinct from Thouless's theorem[16] which states that almost any simple N-particle state $|\Psi\rangle$ can be expressed, to within a complex normalization factor c,

$$|\Psi\rangle = c \exp\left(\sum_{ph} Z_{ph} a^\dagger_p a_h \right) |\Psi_0\rangle , \quad (5.19)$$

where (Z_{ph}) is another set of complex numbers. Thouless's theorem provides an alternative coordinate chart to the one given above; namely, the one given by the real and imaginary parts of (Z_{ph}). One can readily ascertain that this chart also follows from the general construction of Sec. IV by considering Gr_N as an orbit of the general linear

group $GL(\mathcal{H}^{(1)})$ rather than its unitary subgroup as we have done.

Using the above choice of $\bar{k}$ the condition (4.6) that the energy be stationary at Ψ_0 becomes the HF equation

$$\langle\Psi_0|[H, a_p^\dagger a_h]|\Psi_0\rangle = \langle\Psi_0|[H, a_h^\dagger a_p]|\Psi_0\rangle = 0 \tag{5.20}$$

for all $h=1,\ldots,N$, $p=N+1,\ldots,$. Expanding the excitation operators $O_\lambda^\dagger$ of Eq. (4.13):

$$O_\lambda^\dagger = \sum_{p,h} [Y_{ph}(\lambda) a_p^\dagger a_h - Z_{ph}(\lambda) a_h^\dagger a_p] \tag{5.21}$$

we obtain from Eq. (4.14) the RPA eigenvalue equations[1]

$$\sum_{p'h'} [A_{php'h'} Y_{p'h'}(\lambda) + B_{php'h'} Z_{p'h'}(\lambda)] = \omega_\lambda Y_{ph}(\lambda) ,$$
$$\sum_{p'h'} [B^*_{php'h'} Y_{p'h'}(\lambda) + A^*_{php'h'} Z_{p'h'}(\lambda)] = -\omega_\lambda Z_{ph}(\lambda) , \tag{5.22}$$

with the normalization

$$\sum_{ph} [Y^*_{ph}(\kappa) Y_{ph}(\lambda) - Z^*_{ph}(\kappa) Z_{ph}(\lambda)] = \delta_{\kappa\lambda} , \tag{5.23}$$

where

$$A_{php'h'} = \langle\Psi_0|[a_h^\dagger a_p, H, a_{p'}^\dagger a_{h'}]|\Psi_0\rangle ,$$
$$B_{php'h'} = -\langle\Psi_0|[a_h^\dagger a_p, H, a_{h'}^\dagger a_{p'}]|\Psi_0\rangle . \tag{5.24}$$

Finally, Hamilton's equations for the time evolution of an arbitary state on Gr_N become the TDHF equations which are conveniently expressed in density matrix language. We recall the well-known fact that the Grassman manifold Gr_N is diffeomorphic to the set of single-particle density matrices which satisfy the conditions

$$\rho = \rho^\dagger , \quad \rho^2 = \rho, \quad \mathrm{Tr}\rho = N . \tag{5.25}$$

The diffeomorphism is defined as follows: In terms of an orthonormal basis $\{a_\nu^\dagger;\ \nu=1,2,\ldots,\}$ of single-particle creation operators, each $\Psi \in Gr_N$ defines a density matrix with elements

$$\rho_{\mu\nu} = \langle\Psi|a_\nu^\dagger a_\mu|\Psi\rangle . \tag{5.26}$$

One readily ascertains that with Ψ simple, ρ satisfies the conditions (5.25). Conversely, given a density matrix satisfying these conditions, it can be diagonalized by a unitary transformation and, since ρ is idempotent, its eigenvalues can only be zero or one. Thus we can order the eigenvectors such that

$$(U^\dagger \rho U)_{\sigma\tau} = \begin{cases} \delta_{\sigma\tau}, & \sigma=1,\ldots,N \\ 0, & \sigma=N+1,\ldots, \end{cases} . \tag{5.27}$$

The simple state Ψ corresponding to ρ is then defined

$$|\Psi\rangle \equiv a_1^\dagger(U)\cdots a_N^\dagger(U)|-\rangle , \tag{5.28}$$

where

$$a_\nu^\dagger(U) = U a_\nu^\dagger U^\dagger . \tag{5.29}$$

This state is normalized and uniquely defined to within a phase factor.

Since the matrix elements of the density uniquely define the state when it is simple it follows that the set of density matrix elements constitutes a complete set of functions on Gr_N. To define the time evolution of a simple state it is therefore sufficient to define the time evolution of its single-particle densities. The TDHF equation is therefore expressed

$$\dot{\rho}_{\mu\nu} = i\langle\Psi|[H, a_\nu^\dagger a_\mu]|\Psi\rangle . \tag{5.30}$$

It will be shown in the following section that this familiar equation follows in a more general context from Hamilton's equation.

VI. GENERALIZATION OF HARTREE-FOCK CONCEPTS

We have observed that the static HF, RPA, and TDHF theories have counterparts associated with any symplectic submanifold. However, the utility of these generalizations must ultimately depend on the practicality of the theories they generate. It is worthwhile, therefore, to explore in more detail some of the simplifying characteristics of determinant based theories to discover which of them are truly unique and which are amenable to generalization.

One of the obvious characteristics of the HF dynamics is the existence of a HF self-consistent one-body Hamiltonian $h(\Psi)$ defined for each simple state Ψ. This Hamiltonian has the property that the time evolution of the expectation F of any observable F in the constrained HF dynamics (i.e., F a one-body operator) is given by the equation

$$\dot{F} = i\langle\Psi|[h(\Psi), F]|\Psi\rangle . \tag{6.1}$$

We shall show that such a Hamiltonian exists for any symplectic homogeneous space.

Suppose, for simplicity, that M is a symplectic orbit of a unitary group G and that (x^μ) is a coordinate chart induced about a point $\Psi \in M$ by exponentiation of a basis (X_μ) of $\bar{k}$, a vector space complement of the isotropy subalgebra at Ψ in the Lie algebra of G as defined in Sec. IV. The function F, defined on M as the expectation of some observable F, then has time evolution given by

$$\dot{F} = \dot{x}^\mu \frac{\partial F}{\partial x^\mu} = \dot{x}^\mu \langle\Psi|[F, X_\mu]|\Psi\rangle . \tag{6.2}$$

Thus we obtain Eq. (6.1) by defining

$$h(\Psi)=i\dot{x}^{\mu}\mathrm{X}_{\mu}=i\sigma^{\mu\nu}\frac{\partial H}{\partial x^{\nu}}\mathrm{X}_{\mu}\,. \tag{6.3}$$

Alternatively,

$$h(\Psi)=i\sigma^{\mu\nu}\langle\Psi|[\mathrm{H},\mathrm{X}_{\nu}]|\Psi\rangle\mathrm{X}_{\mu}\,.$$

It follows directly from Eq. (4.7) that $h(\Psi)$ has the property

$$\langle\Psi|[h(\Psi),\mathrm{X}]|\Psi\rangle=\langle\Psi|[\mathrm{H},\mathrm{X}]|\Psi\rangle \tag{6.4}$$

for any X in the Lie algebra of G. In fact, this equation defines a convenient intrinsic definition of $h(\Psi)$, which avoids reference to a coordinate chart. Note that, by Eq. (6.3), $ih(\Psi)$ is required to be in the Lie algebra of G and that $h(\Psi)$ is only defined *modulo* an arbitrary and unimportant component from the isotropy subalgebra. One also observes that H Hermitian implies that $h(\Psi)$ is also Hermitian.

Putting Eqs. (6.1) and (6.4) together we obtain the very significant result that

$$\dot{F}=i\langle\Psi|[\mathrm{H},\mathrm{F}]|\Psi\rangle \tag{6.5}$$

for all F in the complexification of the Lie algebra of G. This result is significant because it means that *F takes the same value in the constrained dynamics at any point on* M *as it would have in the unconstrained dynamics*. This result is especially significant for HF theory because the complexification of the one-body unitary Lie algebra is the set of all one-body operators, which includes most of the physical observables of interest. Furthermore, as was shown in the previous section, the expectations of the one-body operators are the one-body densities and these constitute a complete set of functions on the Grassman manifold.

The Hamiltonian $h(\Psi)$ can also be used to give the equation of motion for the time evolution of a state in the constrained dynamics by writing

$$|\dot{\Psi}\rangle=\dot{x}^{\mu}|\partial\Psi/\partial x^{\mu}\rangle=\dot{x}^{\mu}\mathrm{X}_{\mu}|\Psi\rangle\,. \tag{6.6}$$

Thus we obtain the equation of motion for $\Psi(t)$ in the form of a Schrödinger equation

$$h(\Psi)|\Psi\rangle=i|\dot{\Psi}\rangle\,. \tag{6.7}$$

Such an equation is of course very familiar in the TDHF context. It should be emphasized, however, that this equation is not a Schrödinger equation in the usual sense. For whereas the unconstrained Schrödinger equation is a linear equation, the above equation is, in general, nonlinear, which is perhaps not a very surprising outcome in view of the fact that the dynamics has been constrained to a nonlinear space.

Nonlinear differential equations have attracted considerable interest in recent years as a consequence of the discovery that they frequently exhibit nondispersive solitary wave solutions.[17] In the present context the situation is the converse. The suppression of the dispersion of the wave function by constraining the dynamics to a nonlinear space results in a nonlinear equation. Thus the only solutions of Eq. (6.7) of relevance are the nondispersive solutions, i.e., those for which $\Psi(t)$ is a path on the submanifold.

Although it is possible to generalize the definition of $h(\Psi)$ to give the dynamics constrained to an arbitrary symplectic manifold, it would appear to be more useful to work, in general, with the symplectic gradient $\hat{H}$ of the energy function. Associated with any function F on a symplectic manifold M there corresponds a symplectic gradient field

$$\hat{F}=\sigma^{\mu\nu}\frac{\partial F}{\partial x^{\nu}}\frac{\partial}{\partial x^{\mu}}\,. \tag{6.8}$$

This field clearly acts on another function G by

$$\hat{F}(G)=\{F,G\} \tag{6.9}$$

where the curly bracket is the Poisson bracket. The equation of motion for F is therefore given by

$$\hat{H}(F)=\dot{F}\,. \tag{6.10}$$

Another frequently exploited characteristic of the Grassman manifold is the fact that each simple state $\Psi\in\mathrm{Gr}_N$ is a particle-hole vacuum;

$$a_h^{\dagger}a_p|\Psi\rangle=0 \tag{6.11}$$

for some choice of particle-hole operators.[18] This property too is much more general.

If M is an orbit of a semisimple Lie group G and if the orbit contains a lowest weight state Ψ_0 of an irreducible unitary representation of G then the complexification $\tilde{g}^c$ of its Lie algebra $\tilde{g}$ can be decomposed into vector subspaces

$$\begin{aligned}\tilde{g}^c&=\tilde{l}\oplus\tilde{k}\,,\\ \tilde{k}^c&=\tilde{k}^+\oplus\tilde{k}^-\,,\end{aligned} \tag{6.12}$$

where $\tilde{l}$ is the Lie algebra of the isotropy subalgebra at Ψ_0 and $\tilde{k}^-$ is defined such that

$$\mathrm{X}|\Psi_0\rangle=0\,,\quad\text{all}\quad \mathrm{X}\in\tilde{k}^-. \tag{6.13}$$

(Cf. Cartan's decomposition of semisimple Lie algebras.) It follows that every $\Psi\in\mathrm{M}$ is a lowest weight state with respect to some decomposition of $\tilde{g}^c$, i.e.,

$$\mathrm{X}(g)|\Psi(g)\rangle=0\,,\quad\text{all}\ \mathrm{X}\in\tilde{k}^- \tag{6.14}$$

with

$$\mathrm{X}(g)=g\mathrm{X}g^{-1},\quad |\Psi(g)\rangle=g|\Psi_0\rangle\,,\quad g\in\mathrm{G}\,. \tag{6.15}$$

This suggests that among the many possible orbits of a group, those which are lowest weight orbits may be of special significance in many-body applications. One also observes that the elements of such an orbit are generalized Glauber coherent states in the sense of Perelomov and Onofri[19] and that such orbits are naturally amenable to requantization in the coherent-state representation. For example, we have recently shown that the Grassman manifold supports an exact coherent-state representation of many-fermion quantum mechanics.[20]

However, it would appear that the Grassman manifold is exceptional in the sense that it is not only a lowest weight orbit but it has the additional property that every simple state is a vacuum of particle and hole destruction operators separately, i.e.,

$$a_h^\dagger|\Psi\rangle = a_p|\Psi\rangle = 0\,. \tag{6.16}$$

As a consequence, the HF equation (5.20) can be expressed

$$H_{ph}^{(1)} = H_{ph}^{(1)} = 0\,, \tag{6.17}$$

where $H^{(1)}$ is the HF self-consistent-field Hamiltonian with matrix elements defined

$$H_{\mu\nu}^{(1)} = \langle\Psi|\{a_\mu, [H, a_\nu^\dagger]\}|\Psi\rangle\,. \tag{6.18}$$

The significance of this property is that HF solutions can be found by the Hartree self-consistent-field method, i.e., by repeatedly diagonalizing $H^{(1)}$, to determine a single-particle basis in which the off-diagonal particle-hole matrix elements vanish, and then to construct the corresponding particle-hold vacuum as a determinant of occupied hole states. The circumstances under which the Hartree method converges have been investigated recently by two of us.[8]

The variational equation (4.6) for stationary states in general is not, however, a self-consistent-field equation and the Hartree method of solution is therefore not applicable. The equation is nevertheless easily solved by the Newton-Kantorovic method.[9,10] This method is simply a generalization of the familiar Newton method for finding the zeros of nonlinear functions. In the present context, the functions are the components of the energy gradient. The Newton-Kantorovic method will be discussed in some detail in a subsequent paper.[11]

VII. DISCUSSION

The most serious deficiency of the dynamics constrained to a nonlinear symplectic submanifold would appear to be the loss of the superposition principle. However, it is only partially lost. In particular, one observes that the small amplitude normal-mode vibrations about a stable stationary point give linear equations for excited states. These equations correspond to diagonalization of a bilinear form, the Hessian, on a linear space, namely, the tangent space at the stationary point. Nevertheless it remains a fact that two paths on the submanifold corresponding to solutions of the constrained dynamics cannot, in general, be summed to give a third. It is of interest therefore to consider how this limitation might be circumvented.

We have observed that the time evolution of a state constrained to a symplectic homogeneous space is given by a nonlinear Schrödinger equation with a Hamiltonian $h(\Psi)$. An interesting recent suggestion, in the context of TDHF theory, is that one regard the constrained time-dependent wave functions as "channel wave functions" in much the same way that one regards optical-model wave functions for the elastic scattering of various projectiles by a target. Thus one might write the full Hamiltonian

$$H = h(\Psi) + V(\Psi)\,,$$

where $V(\Psi)$ is a residual interaction that couples channels. The construction of an S-matrix theory with TDHF channels is currently being actively pursued.[21]

Another approach to regain a linear theory is that of requantization. This is the approach initiated by Hill, Wheeler, and Griffin.[22] It was observed in Sec. VI that constraining the dynamics to a submanifold can be regarded as a suppression of quantal dispersion effects. And in this sense, the constrained theories can be regarded as semiclassical approximations. For example, the symplectic manifold of Glauber coherent states[23] for a single-particle is diffeomorphic to classical phase space. Now it is well known that the manifold of Glauber coherent states can be requantized to give the Bargmann coherent-state representation[24] which is an exact representation of the single-particle quantum mechanics. In a similar manner we have recently shown that the Grassman manifold can be requantized to give an exact coherent-state representation of many-fermion quantum mechanics.[20] It would of course be unreasonable to suppose that the requantization of an arbitrary symplectic submanifold could give back the full unconstrained quantum mechanics. However, it can be expected to return a linear subquantum mechanics. The general techniques for requantizing arbitrary symplectic manifolds are the topic of intense current activity.[2-4] They would appear to merit investigation in view of the recent interest in constructing fully quantal col-

lective theories by first constructing semiclassical submanifolds on the basis of TDHF or other considerations and then requantizing them.[25] In a following paper we shall extend the above geometric formulation of quantum mechanics to Fock space.

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APPENDIX

Theorem. If $|\Phi\rangle$ is a normalized simple (i.e., Slater determinant) N-particle state and $(a_h^\dagger; h = 1,\ldots,N)$ and $(a_p^\dagger; p = N+1,\ldots,)$ are, respectively, single-particle creation operators for an orthonormal basis of occupied (i.e., hole) and unoccupied (i.e., particle) states defined with respect to $|\Phi\rangle$ as the particle-hole vacuum, then any other normalized simple N-particle state $|\Phi'\rangle$ can be expressed to within a phase factor

$$|\Phi'\rangle \equiv \exp \sum_{p,h} (X_{ph} a_p^\dagger a_h - X_{ph}^* a_h^\dagger a_p)|\Phi\rangle , \tag{A1}$$

where (X_{ph}) is a set of complex numbers.

Proof. Let $(\alpha_h^\dagger; h = 1,\ldots,N)$ be a set of creation operators for an orthonormal basis of single-particle states occupied in $|\Phi'\rangle$. Construct the $N \times N$ matrix

$$n_{hh'} = \langle \Phi | \alpha_h^\dagger \alpha_{h'} | \Phi \rangle , \quad h,h' = 1,\ldots,N . \tag{A2}$$

Since n is Hermitian it may be diagonalized by a unitary transformation. Furthermore, n is positive semidefinite. Thus there exists a basis such that

$$\langle \Phi | \alpha_h^\dagger \alpha_{h'} | \Phi \rangle = n_h^2 \delta_{hh'} . \tag{A3}$$

Let $(\alpha_h^\dagger)$ be such a basis. Then, since

$$[\alpha_h^\dagger, \alpha_{h'}]_+ = \delta_{hh'} , \tag{A4}$$

it follows that the matrix $(\langle \Phi | \alpha_h, \alpha_h^\dagger | \Phi \rangle)$ is also diagonal with elements

$$\langle \Phi | \alpha_h, \alpha_h^\dagger | \Phi \rangle = (1 - n_h^2)\delta_{hh'} . \tag{A5}$$

Now make the expansion

$$\alpha_h^\dagger = \sum_{h'} C_{h'h} a_{h'}^\dagger + \sum_p C_{ph} a_p^\dagger \tag{A6}$$

and define

$$\begin{aligned} n_h H_h^\dagger &= \sum_{h'} C_{h'h} a_{h'}^\dagger , \\ (1 - n_h^2)^{1/2} P_h^\dagger &= \sum_p C_{ph} a_p^\dagger , \end{aligned} \tag{A7}$$

so that we can write

$$\alpha_h^\dagger = n_h H_h^\dagger + (1 - n_h^2)^{1/2} P_h^\dagger . \tag{A8}$$

It follows from (A3) and (A5) that

$$\langle \Phi | H_h^\dagger H_{h'} | \Phi \rangle = \langle \Phi | P_h P_{h'}^\dagger | \Phi \rangle = \delta_{hh'} , \tag{A9}$$

so that $(H_h^\dagger)$ and $(P_h^\dagger)$, whenever they are defined, are creation operators for orthonormal single-particle states, respectively, occupied and unoccupied in $|\Phi\rangle$. Furthermore, if the set $(H_h^\dagger)$ of creation operators which are well defined by Eq. (A7) (i.e., $n_h \neq 0$) is incomplete, it can be completed in an arbitrary way. We may therefore suppose that $(H_h^\dagger; h = 1,\ldots,N)$ is an orthonormal basis for single-particle states occupied in $|\Phi\rangle$.

Now observe that

$$\begin{aligned} \exp[k(P_h^\dagger H_h - H_h^\dagger P_h)] H_h^\dagger \exp[-k(P_h^\dagger H_h - H_h^\dagger P_h)] \\ = (\cos k) H_h^\dagger + (\sin k) P_h^\dagger , \end{aligned} \tag{A10}$$

which by Eq. (A8) gives $\alpha_h^\dagger$ with

$$k = \cos^{-1} n_h . \tag{A11}$$

It follows therefore, since

$$|\Phi'\rangle \equiv \alpha_1^\dagger \cdots \alpha_N^\dagger |0\rangle , \tag{A12}$$

where $|0\rangle$ is the bare-particle-vacuum state, that $|\Phi'\rangle$ can be expressed

$$|\Phi'\rangle \equiv \exp\left(\sum_{h=1}^N \cos^{-1} n_h (P_h^\dagger H_h - H_h^\dagger P_h) \right) |\Phi\rangle , \tag{A13}$$

which is manifestly well defined even when $n_h = 1$ and $P_h^\dagger$ is not defined. Finally, substituting the expansions (A7) for $P_h^\dagger$ and $H_h^\dagger$, gives the desired result (A1). Note that the above is not only a proof of the theorem, it is also a construction of the exponent in Eq. (A1). Furthermore it reveals the extent to which the exponent is unique, i.e., n_h in Eq. (A13) is generically defined uniquely *modulo* 2π.

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