# Nondeterminantal Hartree-Fock theory

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Hartree-Fock (HF) theory is generalized so as to apply to nondeterminantal densities, while retaining the fundamental HF restriction to one-body dynamics. Time development in conventional time-dependent Hartree-Fock and its extension are identical to classical Hamiltonian dynamics.

## I. INTRODUCTION

Hartree-Fock (HF) theory is fundamental among many-body theories for many reasons but perhaps the most significant is the fact that it is a dynamical theory for the one-body density. Since most physical observables, apart from the potential energy, correspond to one-body operators, they are linear functions of the density. Consequently one believes that their time evolutions are reasonably well described in the HF approximation. Unfortunately HF theory restricts the densities to those satisfying the constraints

$$\mathrm{Tr}\rho = A, \quad \rho^2 = \rho . \tag{1}$$

The former, being an expression of particle number conservation, is acceptable. But the latter, which restricts the $A$-fermion wave functions to Slater determinants, is an undesirable constraint. Our objective is to relax this constraint but to retain the essential simplicity of the HF approximation.

Recently we investigated the underlying geometry of the Slater determinants. It was shown that the Slater determinants form a symplectic manifold (phase space) and that the associated Poisson bracket naturally defines a classical Hamiltonian dynamics equivalent to time-dependent Hartree Fock (TDHF). To adopt this geometrical viewpoint, consider the Slater determinants as forming a surface in the many-fermion state space (see Fig. 1). The exact Hamiltonian $H$ may be regarded as a vector field on this surface which is directed, in general, off the surface. The HF Hamiltonian $H_{\mathrm{HF}}$ is the projection of this vector field onto the surface relative to the nondegenerate symplectic form. The TDHF solutions are the integral curves of the HF vector field.

In the preceeding paper, it was shown how to generalize HF concepts to arbitrary symplectic submanifolds of the many-fermion state space. Unfortunately the generalizations usually prove to be too complicated in practical applications. Furthermore, the submanifolds of interest normally prove to be nonsymplectic, so that our generalized dynamics is not well defined. One of the reasons for the excessive complexity is that the many-particle wave function contains much more information than is embodied in its one-body density. We therefore gain much in simplicity by considering only the associated dynamics induced on the one-body densities. What is more, we shall show that the density surfaces are symplectic in all cases, and dynamics is always well defined on them.

In addition to this geometry, there is also an important group structure. The group $U(n)$ of unitary transformations on the $n$-dimensional single-particle space (For simplicity, the single-particle space is assumed to be finite dimensional.) acts transitively on the Slater determinants, i.e., if $\Phi$ is some fixed determinant, then every other determinant is of the form $\hat{g}\Phi$ for some $\hat{g} \in U(n)$. Moreover, as will be shown, this group structure is interrelated with the symplectic geometry since $U(n)$ acts as a group of canonical transformations.

The existence of these interrelated geometric

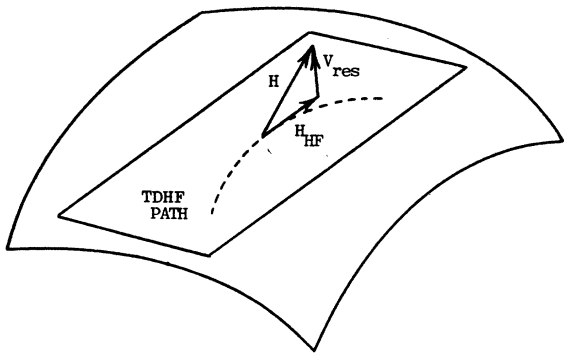


FIG. 1. A TDHF solution drawn as a dotted curve in the surface of determinants. The tangent to this path is the HF Hamiltonian lying in the tangent space. The exact Hamiltonian H and the residual interaction $V_{res}$ are directed off the tangent plane.

and group structures implies an alternative framework for Hartree-Fock theory which enables us to create new generalizations. By the Kostant-Souriau classification theorem for symplectic manifolds with a transitive canonical Lie group action, the Slater determinants must be in one-to-one correspondence with some coadjoint orbit of $U(n)$ (Refs. 2–5). This equivalent statement of Hartree-Fock theory in terms of $U(n)$ coadjoint orbits is nothing other than the familiar density-matrix formulation.[6]

For a fixed, but arbitrary, determinantal density $\rho$, the coadjoint orbit containing $\rho$ is given by

$$\Theta_\rho = \{ g\rho g^{-1} \mid g \in U(n) \} . \tag{2}$$

Every density in this orbit is determinantal and, conversely, every density associated with a Slater determinant is in the orbit $\Theta_\rho$. Indeed, the coadjoint action $\rho \to g\rho g^{-1}$ refers to the transformation in the density induced by a change in single-particle basis associated with $g \in U(n)$. But, every determinant may be obtained from a fixed determinant by a unitary basis transformation.

It is also fruitful to adopt a geometrical viewpoint with the density matrices. Thus, we reinterpret Fig. 1 by considering $\Theta_\rho$, the orbit of determinantal densities, as the surface contained within the space of all possible density matrices, the Hermitian $n \times n$ matrices with trace equal to $A$. A TDHF solution is a curve constrained to the orbit surface and tangent everywhere to the HF Hamiltonian.

Physically, constraint to a $U(n)$ orbit surface means, by definition, restriction to one-body dynamics. This is because the generators of the unitary group are precisely the one-body operators. The crucial point is that this physical interpretation applies not only to the orbit of determinantal densities, but to every $U(n)$ orbit surface. Thus, we are led naturally to consider the continuum of all possible orbits $\Theta_\rho$, each of which defines one-body constrained dynamics. Only one of these surfaces, the orbit $\Theta_\rho$ with $\rho^2 = \rho$, demands that the densities correspond to Slater determinants. The general orbits provide the framework for the desired generalization of conventional TDHF that is investigated in this paper.

The plan of the article is to define the phase-space structure on the generalized orbits in the next section. This symplectic geometry enables us to, first, define classical Hamiltonian dynamics on the orbits and, second, explicitly construct the generalized Hartree-Fock Hamiltonian. In Sec. IV, several ramifications of this generalization are discussed.

## II. COADJOINT ORBITS

A density is fundamentally an element of the dual of the Lie algebra $u(n)$, i.e., a real-valued linear function on the Hermitian one-body operators. Specifically, suppose $\rho$ is the density matrix corresponding to the many-particle state $\Phi$,

$$\rho_{\alpha\beta} = \langle \Phi \mid a_\beta^\dagger a_\alpha \Phi \rangle . \tag{3}$$

A Hermitian one-body operator $\hat{X}$ is defined by a Hermitian matrix $X$ via

$$\hat{X} = \sum_{\alpha\beta} X_{\alpha\beta} a_\alpha^\dagger a_\beta . \tag{4}$$

Then, $\rho$ defines the linear real-valued function of $X$ given by

$$\rho(X) = \langle \Phi \mid \hat{X} \Phi \rangle = \mathrm{tr}(\rho X) . \tag{5}$$

The unitary group transformation of the many-body states $\Phi \to \hat{g}\Phi$ induces the so-called adjoint action on the Lie algebra

$$\hat{X} \to \hat{g}\hat{X}\hat{g}^{-1} \equiv \sum_{\alpha\beta} \mathrm{ad}_g(X)_{\alpha\beta} a_\alpha^\dagger a_\beta , \tag{6}$$

since

$$\begin{aligned} a_\alpha^\dagger(g) &\equiv \hat{g} a_\alpha^\dagger \hat{g}^{-1} = \sum_{\alpha'} a_{\alpha'}^\dagger g_{\alpha'\alpha} , \\ a_\alpha(g) &\equiv \hat{g} a_\alpha \hat{g}^{-1} = \sum_{\alpha'} g^{-1}_{\alpha\alpha'} a_{\alpha'} , \end{aligned} \tag{7}$$

and the adjoint action is defined by

$$\mathrm{ad}_g(X) = gXg^{-1} , \tag{8}$$

for all Hermitian $X$ and $g \in U(n)$. This in turn induces the coadjoint action $\mathrm{ad}_g^*$ on the density matrices

$$\mathrm{ad}_g^*(\rho) = g\rho g^{-1} . \tag{9}$$

As anticipated in Eq. (2), the coadjoint action is compatible with the action of $U(n)$ on the many-particle states,

$$\begin{aligned} \mathrm{ad}_g^*(\rho)(X) &\equiv \langle \hat{g}\Phi \mid \hat{X}\hat{g}\Phi \rangle = \langle \Phi \mid \hat{g}^{-1}\hat{X}\hat{g}\Phi \rangle \\ &= \mathrm{tr}(\rho g^{-1} X g) = \mathrm{tr}(g\rho g^{-1} X) . \end{aligned} \tag{10}$$

Note that in order to use conventional physics terminology, $\rho$ and $X$ are Hermitian, whereas in the mathematical literature the dual elements $\rho$ and Lie algebra elements $X$ are taken to be skew Hermitian. This discrepancy has no deep significance.

The problem now is to characterize the coadjoint orbits $\Theta_\rho$ in a manageable way. First note that each orbit contains a diagonal density $\rho = \mathrm{diag}(\nu_1, \nu_2, \ldots, \nu_n)$, because any Hermitian matrix can be diagonalized by a unitary transformation. Moreover, two distinct diagonal densi-

ties cannot be in the same orbit. Hence, the orbits are enumerated by the set of all $\mathcal{O}_\rho$ as $\rho$ ranges over the diagonal matrices with constant trace equal to $A$. The determinantal densities form the orbit with $\rho = \mathrm{diag}(1, 1, \ldots, 0, \ldots, 0)$; the generic orbits correspond to diagonal $\rho$ with all occupancies $\nu_i$ distinct and $\Sigma \nu_i = A$.

An orbit surface $\mathcal{O}_\rho$ is in one-to-one correspondence with the coset space of $U(n)$ modulo the isotropy subgroup at $\rho$,

$$H_\rho = \{h \in U(n) \,|\, h\rho h^{-1} = \rho\}. \tag{11}$$

To see this, observe that if two group elements $g_1, g_2$ define the same point on the surface $\mathcal{O}_\rho$, $g_1 \rho g_1^{-1} = g_2 \rho g_2^{-1}$, $(g_2^{-1} g_1)\rho(g_2^{-1} g_1)^{-1} = \rho$, or $g_2^{-1} g_1 \in H_\rho$. Hence, by definition, $g_1$ and $g_2$ are in the same coset in $U(n)/H_\rho$, $g_1 H_\rho = g_2 H_\rho$. Thus, the identification of the coset space with the orbit space is given by

$$\begin{aligned} &U(n)/H_\rho \to \mathcal{O}_\rho, \\ &gH_\rho \to g\rho g^{-1}. \end{aligned} \tag{12}$$

For the orbit of determinants, the isotropy subgroup is given by the unitary transformations which separately leave invariant the subspace of occupied hole states and the subspace of particle states. Thus, in this case, $H_\rho = U(A) \times U(n-A)$. For the generic orbits, the isotropy group elements are the pure phase transformations of the single-particle basis $H_\rho = U(1) \times U(1) \times \cdots \times U(1)$ ($n$ copies).

The dimension of the surface $\mathcal{O}_\rho \cong U(n)/H_\rho$ is given by $\dim U(n) - \dim H_\rho = n^2 - \dim H_\rho$. Thus, for the determinantal orbit $\dim \mathcal{O}_\rho = n^2 - [A^2 + (n-A)^2] = 2A(n-A)$, which is twice the number of particle-hole pairs. For the generic orbit, $\dim \mathcal{O}_\rho = n(n-1)$. In every case, the orbit surface is even dimensional.

Geometry on each orbit is determined by the Lie algebra $u(n)$ of the unitary group, the skew-Hermitian $n \times n$ matrices. A basis for this $n^2$ dimensional real Lie algebra is given by the matrices

$$\begin{aligned} &iQ_{\alpha\beta} \equiv i2^{-1/2}(E_{\alpha\beta} + E_{\beta\alpha}), \quad \alpha \geq \beta \\ &iP_{\alpha\beta} \equiv 2^{-1/2}(E_{\alpha\beta} - E_{\beta\alpha}), \quad \alpha > \beta \end{aligned} \tag{13}$$

where $E_{\alpha\beta}$ denotes the $n \times n$ matrix whose sole nonzero entry is one at the intersection of row $\alpha$ with column $\beta$. An arbitrary element $X$ of $u(n)$ is a linear combination of $iQ_{\alpha\beta}$ and $iP_{\alpha\beta}$ with real coefficients. Each such element $X \in u(n)$ defines an element of the group $U(n)$ by exponentiation $\exp X \in U(n)$. Often it is convenient to work with the complexification of $u(n)$ which is spanned by the $E_{\alpha\beta}$, but one must be careful since the connection with the group is lost, $\exp(E_{\alpha\beta}) \notin U(n)$. Fix a diagonal density $\rho$. Each element $X \in u(n)$ defines a curve $\gamma_x(t)$ through the point $\rho$ and lying completely on the surface $\mathcal{O}_\rho$, $\gamma_x(t) \equiv \exp(tX)\rho \exp(-tX)$. The tangent vector to the curve $\gamma_x$ at $\rho$ may be identified with $X$ itself.

Notice, however, that the elements of the isotropy subalgebra $h_\rho$ define zero tangent vectors, since if $X$ is in $h_\rho$, then $\exp(tX)$ is in the isotropy subgroup $H_\rho$ and, hence, $\gamma_x(t) = \exp(tX)\rho \exp(-tX) = \rho$, a fixed point. Thus, the nonzero tangent vectors must correspond to a subspace of $u(n)$ which is complementary to $h_\rho$. There is no unique choice for this complementary subspace, but a convenient selection is given by the subspace $h_\rho^\perp$ orthogonal to $h_\rho$ relative to the Killing form $\kappa$,

$$\text{tan space at } \rho \cong h_\rho^\perp \equiv \{Y \in u(n) \,|\, \kappa(X, Y) \equiv \mathrm{tr}(XY) = 0 \text{ for all } X \in h_\rho\}. \tag{14}$$

For example, in the case of the orbit of determinantal densities, the isotropy subalgebra $h_\rho$ is given by $h_\rho = u(A) \oplus u(n-A) = \mathrm{span}\{iQ_{hh'}, iP_{hh'}\} \oplus \mathrm{span}\{iQ_{pp'}, iP_{pp'}\}$, where $h, h'$ runs over the hole states, the first $A$ vectors, and $p, p'$ runs over the particle states, the last $n-A$ vectors. The orthogonal complement $h_\rho^\perp$ is spanned by the particle-hole matrices $h_\rho^\perp = \mathrm{span}\{iQ_{ph}, iP_{ph}\}$. Thus the dimension of the tangent space is the same as the dimension of the orbit surface $\mathcal{O}_\rho$ itself, viz., $2A(n-A)$. For the generic orbits, the diagonal matrices in $u(n)$ form the isotropy subalgebra, and the tangent space $h_\rho^\perp$ is the skew-Hermitian matrices with every diagonal entry zero.

Consider next the description of the tangent space at an arbitrary point $g\rho g^{-1} \in \mathcal{O}_\rho$. As before, every $X \in u(n)$ defines a curve through that point, viz., $\exp(tX) g\rho g^{-1} \exp(-tX)$. However, the zero tangent vectors are defined now by $X \in g h_\rho g^{-1}$, i.e., $X = gYg^{-1}$, $Y \in h_\rho$. The tangent space at $g\rho g^{-1}$ is identified with the orthogonal complement $(g h_\rho g^{-1})^\perp = g h_\rho^\perp g^{-1}$. Hence, if we set

$$E_{\alpha\beta}(g) \equiv \mathrm{ad}_g(E_{\alpha\beta}) = \sum_{\mu\nu} g_{\mu\alpha} g^{-1}_{\beta\nu} E_{\mu\nu}, \tag{15}$$

then the tangent space at $g\rho g^{-1}$ is spanned by

$$\begin{aligned} &iQ_{\alpha\beta}(g) \equiv i2^{-1/2}[E_{\alpha\beta}(g) + E_{\beta\alpha}(g)], \quad \alpha \geq \beta \\ &iP_{\alpha\beta}(g) \equiv 2^{-1/2}[E_{\alpha\beta}(g) - E_{\beta\alpha}(g)], \quad \alpha > \beta. \end{aligned} \tag{16}$$

Thus, a basis for the tangent space at $g\rho g^{-1}$ is, for the determinantal densities $\{iQ_{ph}(g), iP_{ph}(g)\}$, and for the generic orbits $\{iQ_{\alpha\beta}(g), iP_{\alpha\beta}(g), \alpha > \beta\}$.

In order to complete the geometrical picture, it only remains to define the symplectic structure,

in terms of which the Hamiltonian dynamics is defined in the next section. The symplectic form $\omega$ at the point $g\rho g^{-1}$ in the orbit $\Theta_\rho$ is an antisymmetric form defined on pairs of tangent vectors at $g\rho g^{-1}$,

$$\omega_{g\rho g^{-1}}(X,Y) \equiv -i\,\mathrm{tr}(g\rho g^{-1}[X,Y]), \tag{17}$$

where $X, Y \in u(n)$ are regarded as tangent vectors at $g\rho g^{-1}$. Observe that this definition is consistent with that given in Ref. 1, i.e., if $\rho$ is the density corresponding to the state $\Phi$, then

$$\omega_{g\rho g^{-1}}(X,Y) = -i\langle \hat{g}\Phi | [\hat{X},\hat{Y}]\hat{g}\Phi\rangle . \tag{18}$$

The unitary group action is a canonical transformation on the surface $\Theta_\rho$ because it leaves invariant the symplectic structure

$$\omega_\rho(X,Y) = \omega_{g\rho g^{-1}}(\mathrm{ad}_g(X), \mathrm{ad}_g(Y)), \tag{19}$$

where $X, Y \in u(n)$ are tangent vectors at $\rho$.

At diagonal $\rho$, the form assumes a simple matrix representation in our basis,

$$\begin{aligned} &\omega_\rho(iQ_{\alpha\beta}, iQ_{\alpha'\beta'}) = \omega_\rho(iP_{\alpha\beta}, iP_{\alpha'\beta'}) = 0 , \\ &\omega_\rho(iQ_{\alpha\beta}, iP_{\alpha'\beta'}) = (\nu_\beta - \nu_\alpha)(\delta_{\alpha\alpha'}\delta_{\beta\beta'} - \delta_{\beta\alpha'}\delta_{\alpha\beta'}) . \end{aligned} \tag{20}$$

Therefore, in the ordered basis $\{iQ_{\mathrm{ph}}, iP_{\mathrm{ph}}\}$ for the determinantal orbit,

$$\omega_\rho = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{21}$$

where 0 and $I$ denote the null and identity matrices in $A(n-A)$ dimensions. For the generic orbit in the ordered basis

$$\{iQ_{\alpha\beta}, iP_{\alpha\beta}, \alpha > \beta\}, \quad \omega_\rho = \begin{pmatrix} 0 & D \\ -D & 0 \end{pmatrix}, \tag{22}$$

where 0 and $D$ denote the null and diagonal matrices in $\frac{1}{2}n(n-1)$ dimensions, with $D_{\alpha\beta,\,\alpha\beta} = \nu_\beta - \nu_\alpha$. Since the group action is canonical, the form takes the same matrix representation at every point on the orbit $\Theta_\rho$ in our basis, Eq. (16). An important property of $\omega$ is that it is nondegenerate at every point, i.e., if $\omega_\rho(X,Y) = 0$ for every $Y$, then $X = 0$. This easily follows from the matrix representation.

## III. ONE-BODY DYNAMICS

Because of the symplectic geometry on the coadjoint orbits of densities, we are able now to define one-body dynamics on these orbits. The fundamental approximation is that the time evolution of an initial density $\rho$ is a curve constrained to the orbit surface $\Theta_\rho$. Thus, the tangent vector to each such curve at every point is an element of the unitary Lie algebra; the totality of all such tangent vectors is referred to henceforth as the generalized (density-dependent) Hartree-Fock (GHF) Hamiltonian. We would like to construct the GHF Hamiltonian from the microscopic interaction, as is achieved in conventional Hartree-Fock theory. Indeed, the derivation of the usual HF Hamiltonian by use of the symplectic geometry in the special case of the Slater determinant orbit clarifies the abstract situation considerably.

### A. Orbit of determinants

Suppose $\Phi$ is a determinant and $a_\alpha^\dagger, a_\alpha$ are the associated single-particle fermion operators so that $\rho = \mathrm{diag}(1,1,\ldots,1,0,\ldots,0)$, [cf. Eq. (3)]. At the point $\hat{g}\Phi$, the exact Hamiltonian is regarded as a vector which is not tangent to the orbit surface of Slater determinants, i.e., it defines a curve $\gamma_{\hat{H}}(t) = \exp(i\hat{H}t)\hat{g}\Phi$ of states through the point $\hat{g}\Phi$ which are not in general determinants. On the other hand, the Hartree-Fock Hamiltonian $\hat{H}_{\mathrm{HF}}(\hat{g}\Phi)$ is a vector at $\hat{g}\Phi$ which is, by definition, tangent to the surface and, hence, a one-body operator. Equivalently, because of the one-to-one identification between the orbit of Slater determinants and the orbit of determinantal densities, the HF Hamiltonian is a vector field $H_{\mathrm{HF}}(g\rho g^{-1})$ on the determinantal densities.

The HF Hamiltonian is constructed from the exact Hamiltonian by projection using the symplectic form. Thus, the exact Hamiltonian is the sum of a tangent vector and a residual interaction

$$\hat{H} = \hat{H}_{\mathrm{HF}}(g\rho g^{-1}) + \hat{V}_{\mathrm{res}}(g\rho g^{-1}) , \tag{23}$$

with

$$\omega_{g\rho g^{-1}}(H_{\mathrm{HF}}(g\rho g^{-1}), X) = -i\langle \hat{g}\Phi | [\hat{H},\hat{X}]\hat{g}\Phi\rangle \tag{24}$$

and

$$\langle \hat{g}\Phi | [\hat{V}_{\mathrm{res}}(g\rho g^{-1}), \hat{X}]\hat{g}\Phi\rangle = 0 \tag{25}$$

for every tangent vector $X$ in $u(n)$ at $g\rho g^{-1}$. Since $\omega$ is nondegenerate, Eq. (24) has a unique solution in the tangent space at $g\rho g^{-1}$ given by

$$H_{\mathrm{HF}}(g\rho g^{-1}) = \sum_{\mathrm{ph}} H_{\mathrm{HF}}(g\rho g^{-1})_{\mathrm{ph}} E_{\mathrm{ph}}(g) + \mathrm{H.c.}, \tag{26}$$

where

$$\begin{aligned} H_{\mathrm{HF}}(g\rho g^{-1})_{\mathrm{ph}} &= -\langle \hat{g}\Phi | [\hat{H}, a_h^\dagger(g) a_p(g)]\hat{g}\Phi\rangle \\ &= -\langle \Phi | [\hat{g}^{-1}\hat{H}\hat{g}, a_h^\dagger a_p]\Phi\rangle . \end{aligned} \tag{27}$$

In order to evaluate $H_{\mathrm{HF}}(g\rho g^{-1})_{\mathrm{ph}}$, first write

$$\hat{H}=\sum_{\alpha\beta}T_{\alpha\beta}a_\alpha^\dagger a_\beta+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}V_{\alpha\beta\gamma\delta}a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$
$$=\sum_{\alpha\beta}T(g)_{\alpha\beta}a_\alpha^\dagger(g)a_\beta(g)$$
$$+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}V(g)_{\alpha\beta\gamma\delta}a_\alpha^\dagger(g)a_\beta^\dagger(g)a_\delta(g)a_\gamma(g)\,, \qquad (28)$$

where

$$T(g)_{\alpha\beta}=\sum_{\alpha'\beta'}g^{-1}_{\alpha\alpha'}T_{\alpha'\beta'}g_{\beta'\beta}\,,$$
$$V(g)_{\alpha\beta\gamma\delta}=\sum_{\alpha'\beta'\gamma'\delta'}g^{-1}_{\alpha\alpha'}g^{-1}_{\beta\beta'}V_{\alpha'\beta'\gamma'\delta'}g_{\gamma'\gamma}g_{\delta'\delta}\,. \qquad (29)$$

Then $\hat{g}^{-1}\hat{H}\hat{g}$ is given from Eq. (28) with the substitutions $a_\alpha^\dagger(g)\to a_\alpha$ and $a_\beta(g)\to a_\beta$. After computing the commutator in Eq. (27) and evaluating its expectation value, we find

$$H_{\mathrm{HF}}(g\rho g^{-1})_{ph}=T(g)_{ph}+\sum_{h'}V(g)_{h'ph'h}\,, \qquad (30)$$

which is recognized as the usual Hartree-Fock Hamiltonian derived by other less geometrical methods.[7,8]

### B. Generic orbits

We turn now to the generic orbits and attempt to determine the generalized HF Hamiltonian $H_{\mathrm{GHF}}(g\rho g^{-1})$ employing the same geometrical construction that has proved successful for the Slater determinant orbit. However, a significant modification to the construction is required due to the fact that the map $\hat{g}\Phi\to g\rho g^{-1}$ is a many-to-one correspondence. Indeed every state of the form $\hat{g}\hat{h}\Phi$ for $h\in H_\rho$ is mapped onto the same density $g\rho g^{-1}$. Thus the straightforward generalization of Eq. (24) to the generic orbit is ambiguous. The simplest way to resolve this ambiguity is to average over the states. Thus we generalize Eq. (24) to define $H_{\mathrm{GHF}}(g\rho g^{-1})$ by

$$\omega_{g\rho g^{-1}}(H_{\mathrm{GHF}}(g\rho g^{-1}),X)$$
$$=-i\int_{h\in H_\rho}d\mu(h)\langle\hat{g}\hat{h}\Phi|[\hat{H},\hat{X}]|\hat{g}\hat{h}\Phi\rangle \qquad (31)$$

for every tangent vector $X\in u(n)$ to the orbit $\mathcal{O}_\rho$ at $g\rho g^{-1}$. The measure $d\mu(h)$ on $H_\rho=U(1)\times\cdots\times U(1)$ is the invariant measure,

$$d\mu(h)=\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\cdots\frac{d\theta_n}{2\pi}\,.$$

Since $iH_{\mathrm{GHF}}(g\rho g^{-1})$ is a tangent vector at $g\rho g^{-1}$, we can expand

$$H_{\mathrm{GHF}}(g\rho g^{-1})=\sum_{\alpha>\beta}H_{\mathrm{GHF}}(g\rho g^{-1})_{\alpha\beta}E_{\alpha\beta}(g)+\mathrm{H.c.} \qquad (32)$$

and, by an argument similar to that used in Eqs. (26) and (27)

$$H_{\mathrm{GHF}}(g\rho g^{-1})_{\alpha\beta}=(\nu_\alpha-\nu_\beta)^{-1}$$
$$\times\int_{H_\rho}d\mu(h)\langle\hat{h}\Phi|[\hat{g}^{-1}\hat{H}\hat{g},a_\beta^\dagger a_\alpha]|\hat{h}\Phi\rangle\,, \qquad (33)$$

where $\nu_\alpha$ is one of the distinct entries of the generic diagonal density $\rho=\mathrm{diag}(\nu_1\nu_2,\ldots,\nu_n)$. For the one-body part of $\hat{H}$, the integrand is independent of $h\in H_\rho$ and averaging produces no effect. This reflects the fact that there is no ambiguity in transferring a one-body operator from the orbit of states to the orbit of densities. On the other hand, the two-body part requires averaging. In fact, one encounters integrals of the form

$$\int_{H_\rho}d\mu(h)\langle\hat{h}\Phi|a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta\hat{h}\Phi\rangle\,, \qquad (34a)$$

but, since $h^{-1}a_\alpha^\dagger h=e^{i\theta_\alpha}a_\alpha^\dagger$ and $h^{-1}a_\alpha h=e^{-i\theta_\alpha}a_\alpha$, the integral becomes

$$\int\frac{d\theta_1}{2\pi}\cdots\frac{d\theta_n}{2\pi}\,e^{i(\theta_\alpha+\theta_\beta-\theta_\gamma-\theta_\delta)}\langle\Phi|a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta\Phi\rangle\,. \qquad (34b)$$

Notice that this integral vanishes unless the argument of the exponential is zero. Hence, the integral is evaluated to be

$$(\delta_{\alpha\gamma}\delta_{\beta\delta}-\delta_{\alpha\delta}\delta_{\beta\gamma})\langle\Phi|a_\alpha^\dagger a_\beta^\dagger a_\alpha a_\beta\Phi\rangle\,. \qquad (34c)$$

After computing these two-body averages, the generalized Hartree-Fock Hamiltonian is given by

$$H_{\mathrm{GHF}}(g\rho g^{-1})_{\alpha\beta}$$
$$=T(g)_{\alpha\beta}+(\nu_\alpha-\nu_\beta)^{-1}\sum_\delta V(g)_{\delta\alpha\delta\beta}$$
$$\times\langle\Phi|(a_\alpha^\dagger a_\alpha-a_\beta^\dagger a_\beta)a_\delta^\dagger a_\delta\Phi\rangle\,, \qquad (35)$$

for $\alpha\neq\beta$. This is the desired result.

## IV. DISCUSSION

We have succeeded in constructing a theory of nondeterminantal one-body dynamics. The construction starts with an arbitrary many-body state $\Phi$ and chooses a single-particle basis so that the corresponding density $\rho$ is diagonal. From this, the coefficients

$$R^\delta_{\alpha\beta}=\frac{\langle\Phi|(a_\alpha^\dagger a_\alpha-a_\beta^\dagger a_\beta)a_\delta^\dagger a_\delta\Phi\rangle}{\langle\Phi|(a_\alpha^\dagger a_\alpha-a_\beta^\dagger a_\beta)\Phi\rangle}\,,\quad\alpha\neq\beta \qquad (36)$$

are determined. Then the generalized Hartree-Fock Hamiltonian, a vector field tangent to the unitary orbit of densities $\mathcal{O}_\rho$, is given by

$$H_{\mathrm{GHF}}(g\rho g^{-1})_{\alpha\beta}=T(g)_{\alpha\beta}+\sum_\delta V(g)_{\delta\alpha\delta\beta}R^\delta_{\alpha\beta}\,,\quad\alpha\neq\beta\,. \qquad (37)$$

There are several remarks to be made. First, note that the GHF Hamiltonian reduces to the usual HF Hamiltonian if $\Phi$ is a Slater determinant, since, in that case, $a_\delta^\dagger a_\delta \Phi = \nu_\delta \Phi$ and, hence, $R^\delta_{\alpha\beta} = \nu_\delta$.

Clearly, stationary GHF states are points $g\rho g^{-1}$ on the orbit surface $\mathcal{O}_\rho$ for which

$$H_{\mathrm{GHF}}(g\rho g^{-1})_{\alpha\beta} = 0, \quad \alpha \neq \beta . \tag{38}$$

This may be solved for $g$ by an iterative procedure similar to the Hartree method, or better yet by the Newton method.[9]

Time-dependent GHF solutions are integral curves lying in the orbit surface $\mathcal{O}_\rho$ which are tangent to the GHF Hamiltonian. Therefore, the density $\rho(t) = g(t)\rho g(t)^{-1}$ satisfies the matrix equation

$$\frac{d\rho}{dt} = i[H_{\mathrm{GHF}}(\rho(t)), \rho(t)] \tag{39}$$

or, in terms of $g(t)$,

$$\left(g^{-1}\frac{dg}{dt}\right)_{\alpha\beta} = iH_{\mathrm{GHF}}(g\rho g^{-1})_{\alpha\beta}, \quad \alpha \neq \beta . \tag{40}$$

Observe that this second equation really defines a curve $g(t)H_\rho$ in $U(n)/H_\rho \simeq \mathcal{O}_\rho$. Thus, multiplying $g(t)$ on the right by a diagonal unitary matrix leaves Eq. (40) invariant.

An alternate derivation of the GHF Hamiltonian starts with the energy function on the orbit $\mathcal{O}_\rho$,

$$\mathcal{H}(g\rho g^{-1}) = \int_{H_\rho} d\mu(h) \langle \hat{g}\hat{h}\Phi \,|\, \hat{H}\hat{g}\hat{h}\Phi \rangle . \tag{41}$$

With the energy function defined, Hamiltonian dynamics is immediately determined in a standard fashion.[10] The differential $d\mathcal{H}$ at $g\rho g^{-1}$ is a real-valued form on the tangent space at $g\rho g^{-1}$,

$$d\mathcal{H}(X) = \frac{d}{dt}\,\mathcal{H}(\exp(tX) g\rho g^{-1} \exp(-tX))\big|_{t=0} \tag{42}$$

for every tangent vector $X \in u(n)$. From $d\mathcal{H}$ and the symplectic form $\omega_{g\rho g^{-1}}$, the GHF Hamiltonian is given from

$$\omega_{g\rho g^{-1}}(H_{\mathrm{GHF}}(g\rho g^{-1}), X) = d\mathcal{H}(X) \tag{43}$$

for every tangent vector $X \in u(n)$ at $g\rho g^{-1}$. Using Eqs. (17) and (32) and letting $X = iQ_{\alpha\beta}(g)$ and $iP_{\alpha\beta}(g)$, Eq. (43) may be solved and the GHF Hamiltonian previously derived is recovered.

This alternate derivation is useful because it applies to any energy function $\mathcal{H}$. Thus, if a different choice for $\mathcal{H}$ is made, then Hamiltonian dynamics is still well defined. For example, another sensible choice for the energy is given by

$$\mathcal{H}(g\rho g^{-1}) = \min_{h \in H_\rho} \langle \hat{g}\hat{h}\Phi \,|\, \hat{H}\hat{g}\hat{h}\Phi \rangle . \tag{44}$$

Whether this or our previous expression, Eq. (41), is a better choice for the energy function depends upon both the properties of the state $\Phi$ and the two-body potential $V$. If $\Phi$ is a Slater determinant, then the expectation of $\hat{H}$ is independent of $h \in H_\rho$, and both expressions are identical. In the case when the expectation of $\hat{H}$ is only mildly dependent on $h$, then both energy functions are similar. Because it is easier to compute, the averaged energy is then recommended. On the other hand, if the energy expectation is a strongly dependent function of $h \in H_\rho$ with a sharp deep minimum, then Eq. (44) is clearly more suitable for zero-temperature nuclei. However, at nonzero temperatures, a third choice for $\mathcal{H}$ is presented by weighting the integrand in Eq. (41) with the Boltzmann factor.

It is important to recognize that the exact zero-temperature ground-state density lies on one of the orbits $\mathcal{O}_\rho$. Moreover, its energy is the absolute minimum of Eq. (44) on that surface. Therefore, the search for the ground-state density naturally separates into two different problems: (1) The determination of the surface $\mathcal{O}_\rho$ on which the exact ground-state density lies and (2) the discovery of the minimum minimorum of the energy on that surface.

Finally, when would this generalization of HF be physically appropriate? First, it is the natural extension of the usual HF method for determining the ground-state density. Suppose that a conventional HF calculation has been performed, and it has been discovered that the single-particle energy gap between the two states just above and below the Fermi surface is small. In this circumstance, one does not believe that the HF Slater determinant is a good approximation to the exact ground state. It is then natural to consider, as the next best approximation, the orbit of states formed from the sum of two determinants. The sum of determinants $\Phi$ would then be used to construct $R^\delta_{\alpha\beta}$ and $H_{\mathrm{GHF}}$; the solution $g$ to Eq. (38) defines the best ground state that can be written as the sum of two determinants in the orbit containing $\Phi$. By ranging over all possible sums of two determinants, the best ground state of that form is identified. Of course, it must be a better ground state than the original HF wave function.

A second practical application is to the TDHF explanation of nuclear reactions.[11,12] If the incident and target nuclei are both well described by Slater determinants, then conventional TDHF is perhaps satisfactory. However, if either nucleus cannot be adequately approximated by a Slater

determinant, then conventional TDHF is not physically a well-defined theory. Our new generalization permits an arbitrary initial state $\Phi$ to be selected, although the exit channels are then restricted to be in the same $U(n)$ orbit as the initial state.

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