PHYSICAL REVIEW C VOLUME 21, NUMBER 4 APRIL 1980

Time-dependent–$\mathcal{S}$-matrix Hartree-Fock theory of complex reactions

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(Received 7 February 1979)

Some limitations of the conventional time-dependent Hartree-Fock method for describing complex reactions are noted, and one particular ubiquitous defect is discussed in detail: the post-breakup spurious cross channel correlations which arise whenever several asymptotic reaction channels must be simultaneously described by a single determinant. A reformulated time-dependent–$\mathcal{S}$-matrix Hartree-Fock theory is proposed, which obviates this difficulty. Axiomatic requirements minimal to assure that the time-dependent–$\mathcal{S}$-matrix Hartree-Fock theory represents an unambiguous and physically interpretable asymptotic reaction theory are utilized to prescribe conditions upon the definition of acceptable asymptotic channels. That definition, in turn, defines the *physical range* of the time-dependent–$\mathcal{S}$-matrix Hartree-Fock theory to encompass the collisions of mathematically well-defined "time-dependent Hartree-Fock droplets." The physical properties of these objects then circumscribe the content of the Hartree-Fock single determinantal description. If their periodic vibrations occur for continuous ranges of energy then the resulting "classical" time-dependent Hartree-Fock droplets are seen to be intrinsically dissipative, and the single determinantal description of their collisions reduces to a "trajectory" theory which can describe the masses and relative motions of the fragments but can provide no information about specific asymptotic excited states beyond their constants of motion, or the average properties of the limit, if it exists, of their equilibrization process. If, on the other hand, the periodic vibrations of the time-dependent Hartree-Fock droplets are discrete in energy, then the time-dependent–$\mathcal{S}$-matrix Hartree-Fock theory can describe asymptotically the time-average properties of the whole spectrum of such periodic vibrations of these "quantized" time-dependent Hartree-Fock droplets which are asymptotically stationary on a time-averaged basis. Such quantized time-dependent Hartree-Fock droplet spectra promise the closest analog to the rich array of asymptotic channel eigenstates in the exact Schrödinger theory which single time-dependent Hartree-Fock self-consistent determinants might describe. Whether the time-dependent Hartree-Fock droplets are classical or quantized is determined by the mathematical properties of the periodic solutions of the time-dependent Hartree-Fock equation. If the droplets are in fact classical, then the question remains open whether an explicit requantization, by assumption, could consistently restore the close structural analogy with the exact theory. We argue that if the statistical interpretation of the single determinantal wave function, which is central to the present restructuring of the conventional time-dependent Hartree-Fock description, were to be found inadmissible, then no basis would remain for considering the determinant as a "wave function" in the Schrödinger sense. Finally, we note that the conceptual basis of this time-averaged $\mathcal{S}$-matrix theory need not be restricted to the time-dependent Hartree-Fock theory, but might apply as well to other nonlinear Schrödinger-type models which purport to provide an approximate wave function to describe physical reaction processes.

[NUCLEAR REACTIONS Structural analysis of scattering theory for time-dependent Hartree-Fock single determinantal wave functions; scattering matrix defined as a time average; channels labeled by time-averaged properties of periodic solutions; time-averaged channel orthogonality; classical and quantal time-dependent Hartree-Fock droplets.]

I. INTRODUCTION

A. The numerical time-dependent Hartree-Fock method

The Hartree-Fock, or "average field" method for describing complex systems, either in their stationary states[1,2] or as they evolve in time[3,4] is almost as old as the wave mechanics itself. The practical applications of stationary state Hartree-Fock methods also extend far back in history, and the use of time-dependent Hartree-Fock methods to calculate dynamical features of many-body systems is quite well established.

Within this long history, a novel role has recently been cast for the method with the demonstration[5] that numerical time-dependent Hartree-Fock (TDHF) model calculations for plausibly realistic systems with Skyrme-type forces could be executed in modern computers. Subsequently, the restriction to one dimension[6-8] and to two dimensions[9-11] were overridden, although the practical restriction (arising from the still exhorbitant cost of including six dimensional integrals in the numerical calculation) to radial δ-function forces still remains.[12]

These developments introduced a proliferating technique in the study of complex nuclear systems: the numerical experiment, under which the properties of a complex mathematical system, like the TDHF equations, is studied by calculating numerical results and studying their behavior for clues to the nature of the mathematical system which generated them.[13]

The goal of the present work is to place these numerical experiments into a context appropriate for their interpretation by studying the specific restrictive consequences of the single-determinantal assumption for a wave mechanical reaction theory.

It should perhaps be noted that some of us set out at first with the suspicion that such a gross simplification as the single-determinantal approximation must qualitatively restrict the physical range of the resulting theory, and with the expectation that a valuable service could be performed by listing and studying such deficiencies.[14] Such an attitude is not uncommon among researchers in the field, although sometimes it is stated more obliquely as in the claim that TDHF is a "classical" theory, or in the expectation that TDHF can describe only mean values of such quantities as fragment excitation energies.

However, we set for ourselves the requirement that our criticism has also to be sharp and specific, a requirement which turns out to be a substantial burden. Not surprisingly, for one must expect that families of systems might be constructed such that the Hartree-Fock approximation improves monotonically with certain variable parameters (such as, e.g., the range of the two-body interaction), offering prospective counterexamples to any too broad a claim of deficiency. Thus any valid criticism must somehow either incorporate or elude such specific properties. As a result, we found that specific proof of qualitative deficiency is not easy to marshal against TDHF.

Nevertheless, there emerged one ubiquitous qualitative flaw in the TDHF reaction theory: the occurrence of post-breakup spurious cross channel correlations (Sec. III), which *always* occur whenever a single determinant is obliged to describe many reaction channels. This deficiency must therefore as a matter of principle afflict any attempted description of a multichannel reaction by the conventional initial-value TDHF description. (Note that this is a difficulty essentially related to the theory as a *reaction* theory, and is irrelevant for any application involving only bound states.) Moreover, even this difficulty, we found can be circumvented within the single-determinantal restriction, but only by a complete restructuring of the conventional initial-value theory, which we refer to as the time-dependent-$\mathcal{S}$-matrix Hartree-Fock (TD-$\mathcal{S}$-HF) theory.[15-18]

TD-$\mathcal{S}$-HF takes the single-determinantal restriction to comprise the essential element of the TDHF method. From such a viewpoint the TDHF equation is a dynamical system analogous with the time-dependent Schrödinger equation (albeit approximately), capable of generating a time-dependent solution for every possible initial condition (within its determinantal restriction). Then one is led to a sharp structural question: How does the restriction to single determinants alter the qualitative structure of the TDHF reaction theory as compared with the Schrödinger asymptotic reaction theory? This question then emerges as the main target of the present research.

We find that the answer lies in still unknown properties of the TDHF periodic solutions. In particular, a remarkably complete analogy to the Schrödinger reaction theory can be realized within the dynamics of single determinants if (a) periodic solutions to the nonlinear TDHF equation are allowed to play the role of stationary Schrödinger solutions, and if (b) the spectrum of periodic TDHF solutions is discrete in energy. The resulting theory, however, predicts measurements only of time-averaged properties of the periodic solutions, which here substitute for the eigenvalues which characterize the asymptotic eigenstates of the exact Schrödinger theory.

Otherwise the content of the TDHF reaction theory is seriously restricted by the nonorthogonality of energy-degenerate asymptotic states. It can then describe trajectories, but provides no information on the internal states of the emergent droplets, apart from average values of asymptotically conserved quantities such as energy and angular momentum.

Thus, although TDHF is surely not an exact theory, it may nevertheless be recast into a structurally faithful image of the exact theory, provided the (still unknown) properties of its periodic spectrum are suitable.

In Sec. II we review the bases of the conventional TDHF numerical method, noting the economy of its (single) assumption and the remarkable range of qualitative features of nuclei[18] which that assumption incorporates.

In Sec. III we outline briefly the several ways in which, for all its economy and appropriateness, conventional TDHF is an *approximate* theory.[14] Of these we focus in Sec. IV on one,[19,20] the interpretation of the postbreakup asymptotic phase, and especially the postbreakup spurious cross channel correlations which it, inevitably, involves.

In Sec. V a restructuring of the single-determinantal assumption is developed, the TD-$\mathcal{S}$-Matrix HF method, which succeeds in eliminating the post-breakup spurious cross channel correlations, and expands the theory by introducing many wave functions while still remaining within the single-determinantal assumption for each wave function and the self-consistent Hartree-Fock description of its time evolution (considered as Axiom I of the theory). This method focuses upon overlap amplitudes,[21-28] $\langle\Phi_f|\Phi_i\rangle$, among the single-determinantal solutions allowed in the theory as fundamental for extracting its physical content. Indeed this statistical interpretation of the determinantal wave amplitudes, which are here to be interpreted on the time average, comprises Axiom II of the present theory.

In Sec. VI, two *minimal* requirements are ascertained for the TD-$\mathcal{S}$-HF theory (or for any time-dependent theory) to provide an asymptotic description of reaction processes analogous to that of the exact Schrödinger theory. The implications of these requirements for the exhaustive labels which can specify final state reaction channels in the single-determinantal, self-consistent time-dependent framework are extracted. One finds that these *minimal* requirements can be satisfied by requiring the channels to describe stationary Hartree-Fock solutions, and (provided the measurements predicted by the theory are stipulated to be time-averaged measurements) periodic TDHF solutions for each emergent fragment. Then the theory describes the collisions of mathematically well-definable objects which we refer to as "TDHF droplets." The corresponding asymptotic reaction channel states are associated one to one with the periodic[29] TDHF vibrations of the isolated droplets.

In Sec. VII, the properties of the TDHF droplets and their reaction channels are discussed. In particular, the close interrelationship between the consistent application of the statistical interpretation and the mutual orthogonality of the reaction channels is analyzed in detail. The result is that mutual channel orthogonality, on a time-averaged basis, is, or is not, a property of the theory depending on whether the periodic spectrum is, or is not, discrete in energy. Thus two qualitative possibilities emerge: (a) the *continuous* periodic energy spectrum, which we show implies "intrinsically dissipative" TDHF droplets, and allows only a "trajectory" theory, describing asymptotically only the realtive motion of "thermalized" droplets; (b) the *discrete* periodic energy spectrum, for which the theory can predict reaction amplitudes to each member of the discrete set of asymptotic reaction channels, in full analogy with the exact Schrödinger reaction theory.

Section VIII discusses the general bases for the central assumption of the theory (Axiom II) that the wave function, during each instant of time in the interaction interval, obeys the statistical assumption of quantum mechanics as regards the transition amplitude to other states, which evolve into the future along different dynamical trajectories. The implication is emphasized that the whole TDHF method would be discredited as a proper quantum reaction theory, if this statistical interpretation were shown to be inadmissible.

In Sec. IX the application of this statistical interpretation to the TDHF wave functions in the TD-$\mathcal{S}$-HF method is seen to depend not at all upon the specific properties of single-determinantal wave functions. Therefore, one concludes that it offers prospect of application to a class of nonlinear models which provide an approximate time-dependent Schrödinger wave function and have solutions which satisfy certain periodicity and translational properties. At this level of abstraction, the present method is seen to circumvent the difficulties which follow from the loss of the superposition principle by a careful selection of acceptable continuum states to which the statistical interpretation of quantum mechanics shall apply.

Section X summarizes the results and conclusions of this work.

II. CONVENTIONAL INITIAL-VALUE TIME-DEPENDENT HARTREE-FOCK THEORY

We consider the numerical time-dependent Hartree-Fock method[5,13] which so economically and completely incorporates the qualitative features of Nuclear Fermidynamics[16,18] into the single assumption that the exact solution, Ψ, will be approximated as

$$\Psi \sim \Phi\,, \tag{1}$$

a single determinant. This assumption, imposed as a restriction on the same variational principle whose *unrestricted* variation yields the time-dependent Schrödinger equation

$$(H - i\hbar\partial/\partial t)\Psi = 0 \tag{2}$$

leads to the *constant-$\langle\mathcal{H}\rangle$ Hartree-Fock-equation*,[30,31]

$$\mathcal{H}[\Phi]\Phi = (\mathcal{H}^{\mathrm{HF}} - \langle\mathcal{H}^{\mathrm{HF}} - H\rangle)\Phi = i\hbar\partial/\partial t\,\Phi \tag{3}$$

to describe the time evolution of the determinantal wave function. Then, the statement that

$$\Phi(t)|_{t=t_i} = \Phi_0\,, \tag{4}$$

specifies the initial condition, whence Eq. (3) determines[32-39] the solution $\Phi(t)$ for all subsequent times.

Within its single-determinantal assumption the TDHF method incorporates several qualitative features remarkably appropriate for nuclear systems.[16,18] In particular, it describes small, finite, and self-bound systems; it seems to allow very naturally for initially very disequilibrized states, and for substantial matter flow, and the consequent (sometimes qualitative) global alteration of the self-consistent nuclear field. Thus it offers promise of structural relevance to the long mean free path of nucleons inside the nucleus[40-47] (which property follows from the Pauli exclusion principle and allows the shell model behavior of nuclei to occur[48,49]); to the distinctly finite number of nucleons in the nucleus, and the consequent granularity of their single-particle spectra (which properties leads to Strutinsky[50] corrections of the collective potential energy surfaces[50-54] and to corresponding structure in inertial[55-57] and presumably, the dissipation parameters[16,18]); and to the strong equilibrization tendency which is guaranteed by the initial conditions of the heavy ion reaction problem.[58] In addition, the method is constructed specifically to describe the self-bound property which nuclei share, and the response of the average field to matter flow.

We emphasize that the successful incorporation of these several important qualitative physical features into the concise assumption that the wave function is a single determinant, which the time-dependent Hartree-Fock method achieves, is no assurance that the resulting description will adequately describe observed nuclear data. Indeed, the principle of commensurability[59] might on general grounds dim one's hope to get so much from so little (and in Sec. IV we focus upon one specific deficiency of this assumption).

Even so, the TDHF is of great interest, precisely because of the very economy of its assumptions, as a theorist's theory, to teach one how to look at problems in Fermidynamics[18] and what reasonably to expect from them. For this reason alone, even if no expectation whatsoever of immediate meaningful confrontation between TDHF and observed data existed, the properties of the single-determinantal assumption would still deserve study.

III. APPROXIMATE ASPECTS OF THE CONVENTIONAL NUMERICAL TDHF METHOD

We emphasize that in spite of the remarkable incorporation of the main qualitative nuclear properties into the TDHF method (as exhibited in Table I[60-63]), the method is still an *approximate* method. Its restriction to a single determinant limits the accuracy of TDHF in each of the three aspects of its time-dependent description[14]:

(i) The specification of the initial wave function $\Psi_i(t_i)$ by a single-determinant approximation is (generally) inexact, and inflexible.

(ii) Its propagation forward in time to and through the collision by $\mathcal{H}^{HF}$ instead of H_{EXACT} is approximate (omitting, e.g., some two-nucleon correlations). Furthermore, the variational

TABLE I. Time-dependent Hartree-Fock compared with others. Six physical features of relevance to nuclei are tabulated against four theoretical approaches to the nuclear heavy-ion problem. The entries Yes or No indicate whether each of the theoretical approaches specifically incorporates the given property mechanistically into its description. The Table shows that the single-determinantal theory succeeds exceptionally well in incorporating all of these qualitative features into its very succinct single-determinantal assumption. This table is discussed more extensively in Ref. 18. Other references relevant to the theories mentioned are as follows: for A Refs. 1–11, for B Refs. 60 and 61, for C Refs. 62 and 63, and for D Ref. 47.

	Theory			
Physical property	A. Time-dependent single-determinantal theory	B. Navier-Stokes hydrodynamics	C. Fokker-Planck transport theory	D. Wall formula for one-body dissipation
1. Small Fermi ($\lambda > R$)	Yes	No	No	Yes
2. Finite-A (generalized shells)	Yes	No	No	No
3. Liquid (self-bound)	Yes	Yes	No	No
4. BCS paired	Yes (TDHFB)	No	No	No
5. Global, mass-dynamical	Yes	Yes	No	No
6. Non-equilibrium dissipative	Yes (?)	Yes	Yes	Yes

principle from which it flows is unsupported by any concavity theorem,[64-66] which provides a qualitative guarantee that the restricted minimization of the variational integral actually optimizes the quality of the solution.

(iii) The postbreakup determinant, $\Phi(t)$ $(t \gg 0)$, is too simple to describe the many channels of the exact outgoing state, and to date lacks even a specific proposal for an exhaustive physical interpretation.

Some previous effort has been directed at the propagation approximation (ii) of TDHF in the form of studies of the deviation of the exact solution from the TDHF determinant (assumed exact initially) as time progresses,[14,19,20] and of the time evolution of average values of certain operators under TDHF.[67]

IV. POST-BREAKUP SPURIOUS CROSS CHANNEL CORRELATIONS

Here we focus upon the third approximate aspect of TDHF and upon a remedy for the specific incommensurability between the single TDHF determinant and the outgoing multichannel state of the true Schrödinger system. In particular, we argue that, after the collision and breakup into two spatially separate densities, the TDHF wave function involves *spurious cross channel correlations,* because it attempts to describe a "coherent superposition of outgoing channels." The available reaction channels correspond to different pairs of nuclei and a range of possible excited states for each pair, which, if they were allowed to propagate independently, would surely be found at large distances to be separating with a variety of relative velocities. But in TDHF only one mean relative velocity (that prescribed by the relative velocity of the separating potential wells) enters, even though the wave function must purport to describe all channels.

We show now that the single-determinantal limitation of the Hartree-Fock description and the consequent calculation of the single self-consistent potential by means of a single determinant, result, for a multichannel situation, in contributions to the potential energy which do not occur in the asymptotic channels of the exact linear Schrödinger theory and which, therefore, we label "spurious."[68,69] These spurious interactions exert a distorting influence on the physical content of the final stage of the description—a stage which ought to be very simple since it need describe merely the translation in space of the well-separated fragments which have been formed from the reaction process.

To elaborate, imagine $\Phi(t)$ of the time-dependent Hartree-Fock description to be expanded in a complete set of exact channel wave function Ψ_f for the Schrödinger problem:

$$\Phi(t)=\sum_f c_f \Psi_f(t) \quad \text{for} \quad t \gg 0 . \tag{5}$$

(Never mind there the complication that the coefficients c_f certainly depend on time.[70]) In particular, if the reaction were initiated as $^{16}\mathrm{O}+{}^{16}\mathrm{O}$, then one label f should denote, e.g., the $^{28}\mathrm{Si}+{}^{4}\mathrm{He}$ channel. Then consider the (direct term of the) Hartree-Fock potential

$$V_{\mathrm{HF}}(\vec{r})=\int V(\vec{r}_1-\vec{r}_2)\rho(\vec{r}_2)d^3\vec{r}_2 \tag{6}$$

$$=|w_{\mathrm{O-O}}|^2 V_{\mathrm{HF}}^{\mathrm{O-O}} + |w_{\mathrm{Si-He}}|^2 (V_{\mathrm{HF}}^{\mathrm{Si-He}}+V_{\mathrm{HF}}^{\mathrm{He-Si}})+\cdots . \tag{7}$$

Here $V_{\mathrm{HF}}^{\mathrm{O-O}}$ denotes the one-body potential, which would result from averaging the two-body interactions over the exact wave function describing two $^{16}\mathrm{O}$ nuclei, well separated in space. Similarly, the $V_{\mathrm{HF}}^{\mathrm{Si-He}}$ is the one-body potential obtained from the exact wave function, describing $^{4}\mathrm{He}$ and $^{28}\mathrm{Si}$, moving apart each in some particular excited state. Other terms occur for every possible pair of excited states in every possible pair of fragments. Equation (7) demonstrates the fact that *the Hartree-Fock potential, even in the asymptotic region, is (or ought to be) a mixture of potentials for the several channels it attempts to describe.* It cannot, therefore, be the Hartree-Fock self-consistent potential *for any single channel.*

A very similar argument shows that only those selected channels which *happen to have* the same mean relative velocity as the separation velocity of the two parts of the Hartree-Fock potential can have even a possibility of adequate description by the conventional TDHF. The Hartree-Fock propagation preserves the average total energy, the average total momentum, and the total nucleon number; thus, the expectation values,

$$E=\langle\Phi|H_{\mathrm{EX}}|\Phi\rangle , \tag{8}$$

$$\langle\vec{P}\rangle=\langle\Phi|\sum_{i=1}^{A}\vec{p}_i|\Phi\rangle , \tag{9}$$

$$A=\sum_{i=1}^{A}\int d\vec{r}\langle\Phi|\delta(\vec{r}-\vec{r}_i)|\Phi\rangle , \tag{10}$$

are constants in time. (See the Appendix.) For the late stages of a TDHF process when Φ is nonzero only in two well-separated finite volumes, the expression (8) separates into the sum,

$$E=E_1+E_2=T_1+E_1^*+T_2+E_2^* , \tag{11}$$

where T_1 and T_2 represent the translational kinetic energy of the two separate fragments, given in terms of their mean velocities $\vec{v}_1$ and $\vec{v}_2$ by

$$T_1=\tfrac{1}{2}MA_1\vec{v}_1^{\,2}\,,\quad T_2=\tfrac{1}{2}MA_2\vec{v}_2^{\,2}\,, \tag{12}$$

and E_1^* and E_2^* describe their respective internal energies. M is the nucleonic mass. But momentum and nucleon conservation prescribe one kinetic energy in terms of the other:

$$T_2=(A_1/A_2)T_1\,. \tag{13}$$

Therefore, energy conservation together with (13) implies that, asymptotically, the total internal excitation energy

$$E^*=E_1^*+E_2^*=E-(T_1+T_2)\,, \tag{14}$$

is fixed uniquely by the asymptotic values of one fragment mass, and one fragment velocity, A_1 and $\vec{v}_1$. Thus we conclude that only those channels whose excitation energy happens to conform with the asymptotic separation velocity and mass split of the late-time TDHF wave function Φ can have significant nonzero amplitudes in the conventional TDHF description. Obviously no such restriction applies to final channels of the exact Schrödinger theory, each of which asymptotically is described by its own "channel Hamiltonian" to an arbitrarily good approximation.

We conclude from the existence of these spurious cross channel correlations in the late stages of a multichannel process as described by TDHF, that the TDHF description, as conventionally applied, enhances certain channel amplitudes for physically irrelevant reasons and, therefore, is not able to describe the self-consistent propagation in time of *any one* of several outgoing open channels in the final stages of a reaction process. Only in the trivial case of a collision involving one single outgoing channel can the outgoing TDHF state provide the best single-determinantal description of that particular pair of separating fragments.

From these considerations we are led to propose the following heuristic reformulation of the conventional TDHF description—the TD-$\mathcal{S}$-HF description—which obviates these spurious cross channel correlative effects in the final stages of the reaction. In the process, we identify and discuss two basic axioms from which the theory logically flows.

V. THE TIME-DEPENDENT-$\mathcal{S}$-MATRIX HARTREE-FOCK DESCRIPTION OF MANY-PARTICLE REACTIONS

A. Single-determinantal axiom

We consider a theory in which every allowable wave function is a single determinant whose evolution in time obeys the fundamental axiom of the TDHF method,

$$\text{Axiom I:}\quad \mathcal{H}[\Phi(t)]\Phi(t)=i\hbar\dot{\Phi}(t)\,. \tag{15}$$

We first make a simple renotation of the time-dependent Hartree-Fock solutions of (15) evolved from the initial state i by the Hartree-Fock propagation forward in time. Let

$$\Phi(t)=\Phi_i^{(+)}(t)=U_i^{(+)}(t,t_i)\Phi_i^0(t_i)\quad (t\geq t_i) \tag{16}$$

be the familiar TDHF solution, where the propagator U_i represents the (nonlinear) Hartree-Fock process of propagating the wave function Φ_i^0 forward in time from the initial time t_i to the later time t. Analogously, we define the wave function

$$\Phi_f^{(-)}(t)=U_f^{(-)}(t,t_f)\Phi_f^0(t_f)\quad (t\leq t_f) \tag{17}$$

to be the wave function obtained via the TDHF process by stepping backwards in time from t_f to t beginning with $\Phi_f^0(t_f)$.

B. The (time-dependent) $\mathcal{S}$ matrix

We then construct the following analog of the scattering matrix[25,26]:

$$\mathcal{S}_{fi}(t)=\langle\Phi_f^{(-)}(t)\,|\,\Phi_i^{(+)}(t)\rangle\,. \tag{18}$$

Were the wave functions $\Phi_f^{(-)}$ and $\Phi_i^{(+)}$ to be replaced by the exact solutions, $\Psi_f^{(-)}$ and $\Psi_i^{(+)}$, to the Schrödinger equation, this integral would yield the S-matrix element,[25-27]

$$S_{fi}=\langle\Psi_f^{(-)}\,|\,\Psi_i^{(+)}\rangle\,, \tag{19}$$

which gives the amplitude for the wave packet evolved from the initial state i to be found at time t in the state $\Psi_f(t)$ which evolves in time into the asymptotic channel state defined by the simple late-time boundary conditions f. In the exact theory, since the solutions are evolved in time by the exact Hamiltonian H, it is guaranteed that S_{fi} in (19) is a constant independent of time.

Unfortunately, the TDHF S-matrix analog of (18) is surely not a time-independent quantity, since its time derivative, given by Eq. (3),

$$\dot{\mathcal{S}}=d\mathcal{S}_{fi}/dt=(i/\hbar)\langle\Phi_f^{(-)}(t)\,|\,\mathcal{H}^\dagger(\Phi_f)-\mathcal{H}(\Phi_i)\,|\,\Phi_i^{(+)}(t)\rangle \tag{20}$$

is not identically equal to zero. Although in some special cases, $\dot{\mathcal{S}}_{fi}$ may be small or zero (e.g., when $f=i$), there appears no way to guarantee this in general.

Indeed, Eq. (20) must be expected frequently to be at least as large as typical matrix elements of the two-body force such as occur, e.g., in nuclear pairing theory. These have magnitude $\sim 20/A\approx 0.1$ MeV, and would imply for $\dot{\mathcal{S}}$ a value $\sim 10^{20}$/sec.

Furthermore, one must anticipate that in the highly excited states to be treated in TDHF theory, scatterings may occur between single-particle states localized in some nuclear subvolume, leading to a reduction of the volume-proportional denominator A_1 in the two-body matrix element, and a corresponding increase in $\dot{\mathcal{S}}$, perhaps to a value as large as 10^{22}/sec.

It follows that $\mathcal{S}(t)$ may vary significantly during the interaction interval T_{int} of a nuclear heavy-ion reaction,[71] $10^{-22} < T_{\text{int}} < 10^{-20}$/sec. Thus, one is precluded from attaching to the TDHF $\mathcal{S}$ of (18) any general interpretation by direct analogy with the Schrödinger S matrix (19). One might at this stage despair that any semblance of the Schrödinger reaction theory structure can survive the single-determinantal approximation; at the very least, one is forced to consider drastic measures to save some plausible interpretability for the theory.

C. Time-averaged $\bar{\mathcal{S}}$

We adopt an optimistic point of view and assume that even if the $\mathcal{S}$ matrix at no particular instant of time describes the whole reaction process, nevertheless some appropriate time average of $\mathcal{S}$ during the interaction interval might still offer physical content. We therefore interpret $\mathcal{S}_{fi}(t)$ to be the instantaneous amplitude that the TDHF "state" $\Phi_i^{(+)}(t)$ is found at time to be the TDHF state $\Phi_f^{(-)}(t)$, which will *evolve under TDHF to the final state* Φ_f^0 *at* $t = t_f$, *without post-breakup spurious cross channel correlations with other channels*. The total (relative) amplitude that the asymptotic channel state f is realized is taken to be the integral of this amplitude over some interval to be specified more precisely below. Then we propose that

$$\bar{\mathcal{S}}_{fi} = (T_2 - T_1)^{-1} \int_{T_1}^{T_2} dt' \mathcal{S}_{fi}(t') \tag{21}$$

describes, for properly chosen values of T_1, T_2, the (relative) amplitude that the TDHF state i, which evolves from Φ_i^0 at $t = t_i \ll 0$, will be found in the state Φ_f^0 at $t = t_f \gg 0$.

We note that such an averaging process leads for an $\mathcal{S}$-matrix element which is constant over the averaging interval to an $\bar{\mathcal{S}}$-matrix element of precisely the same value. In particular, if Φ_i and Φ_f were to be exact solutions of the Schrödinger equation, then $\mathcal{S}_{fi}$ would reduce to the exact S-matrix amplitude (19). Note also that after (T_1, T_2) have been specified as below, $\mathcal{S}_{fi}$ depends

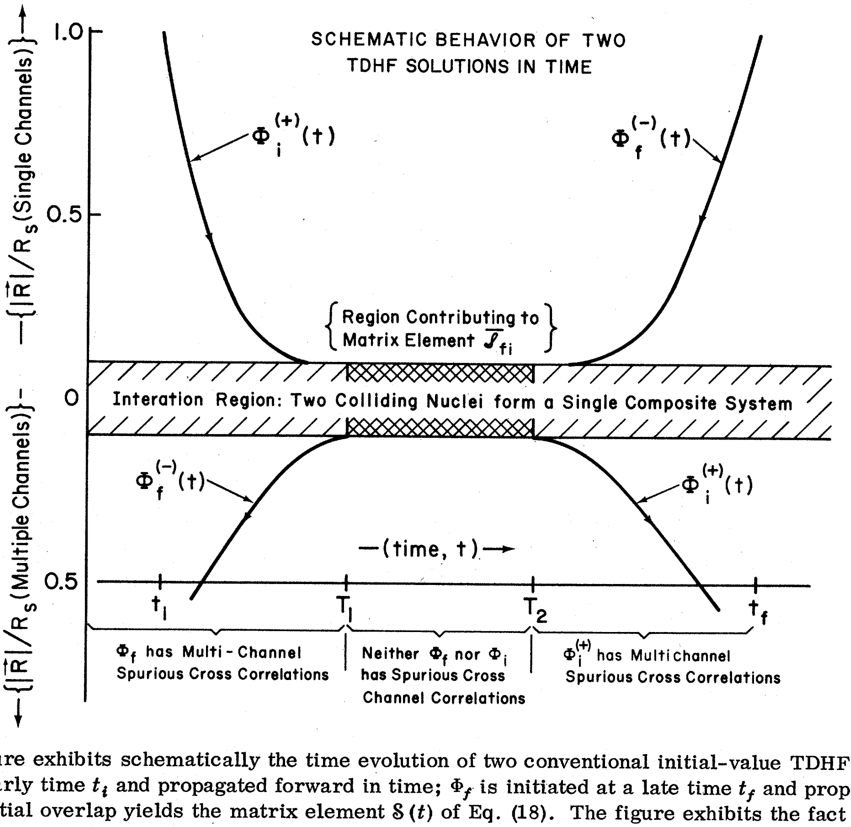

FIG. 1. This figure exhibits schematically the time evolution of two conventional initial-value TDHF solutions. Φ_i is initiated at an early time t_i and propagated forward in time; Φ_f is initiated at a late time t_f and propagated backwards in time. Their spatial overlap yields the matrix element $\mathcal{S}(t)$ of Eq. (18). The figure exhibits the fact that only during the interval (T_1, T_2) are these functions both free of post-breakup spurious cross channel correlations. Distances are scaled against R_s, the chosen (large) standard distance at which, by convention, all reactions are initialized.

not upon t_f and t_i separately, but only upon their difference, $t_f - t_i$. (See also Sec. VIK below.)

D. Specification of limits T_1, T_2 in $\mathcal{S}$-matrix integration

Regarding the choice of the limits in integral (21), we adopt a mechanistic view of the TD-$\mathcal{S}$-HF theory: that it is designed to eliminate from the physical implications of the theory any influence of Hartree-Fock wave functions which involve spurious cross channel correlations in the post-breakup region. In fact, both $\Phi_i^{(+)}$ and $\Phi_f^{(-)}$ involve such spuriousity at very late and very early times, respectively. (See Fig. 1.) Thus, the earliest limiting time T_1 is given by the time at which $\Phi_f^{(-)}$ in its backward evolution in time redisintegrates into two fragments. Likewise, the latest limiting time T_2 is given by the time at which $\Phi_i^{(+)}$ redisintegrates. Then at no time during the whole interval over which $\bar{\mathcal{S}}$ is calculated is either wave function subject to errors induced by post-breakup spurious cross channel correlations.

E. Axiomatizing the statistical interpretation of Φ

Although Eq. (21) arose pragmatically from the effort to extract a physically meaningful reaction amplitude, it can be premised more fundamentally on the general requirement that if a determinant Φ is to be properly considered as a quantum probability amplitude, then the statistical interpretation[21-28] of the quantum theory must be applicable to it. Thus we postulate Axiom II: The spatial integral,

$$\langle \Phi_f | \Phi_i \rangle = a_{fi}\,, \tag{22}$$

defines the amplitude that Φ_i be found in the state Φ_f. Then the quantity $\bar{\mathcal{S}}$ in (21) is the average of the amplitude that Φ_i be found to be Φ_f during the interval (T_1, T_2) when neither Φ_i nor Φ_f suffers spurious cross channel correlations.

We note that if the statistical interpretation of Φ_i had to be rejected, then the operational implications of calling Φ a "quantum wave function" would have been nullified. It would then follow that TDHF was in fact not at all a quantal (in the Schrödinger sense) theory of probability *amplitudes*, but (at best) some classical theory of probabilities cast in the familiar, but misleading, Schrödinger-like form.

Since our analysis is designed to define the broadest possible scope for the single-determinantal TDHF simplification of the Schrödinger theory, we here (and elsewhere in this work) *assume* that the theory is a quantal theory until the contrary is established. Therefore we proceed assuming a plausible quantal interpretation, and trace out the theoretical consequences. Then consistency will require that Axiom II be invoked for *any* pair of wave functions which occur in the theory. Indeed, we shall see that such a consistent application of this axiom to the asymptotic reaction "channels" compels (in Sec. VI) qualitative implications for the physical content of the theory, and most especially the general conclusion that in the single-determinantal reaction theory only time-averaged amplitudes are susceptible to physical interpretation analogous to that of the exact Schrödinger amplitudes.

F. Unitarity and conservation of probability

In the Schrödinger theory, the S matrix is unitary, and time independent, and therefore the total normalization (i.e., the summed probability that the system is found in some state) remains constant in time. But under Axiom I, the TDHF determinants propagate in time each under its own separate time-dependent Hartree-Fock "Hamiltonian." As a result, $\bar{\mathcal{S}}_{fi}$ in (21) is *not* unitary, and conservation of probability does not follow automatically.

We *impose* the conservation of probability by renormalizing $\bar{\mathcal{S}}_{fi}$ into

$$\hat{\bar{\mathcal{S}}}_{fi} = \bar{\mathcal{S}}_{fi} \Big/ \left[\sum_f \bar{\mathcal{S}}_{fi}^* \bar{\mathcal{S}}_{fi} \right]^{1/2} \tag{23}$$

for each initial channel and interpreting $\hat{\bar{\mathcal{S}}}_{fi}$ as the operational analog of the unitary S matrix in the TD-$\mathcal{S}$-HF theory. Equation (23) completes the required reformulation of the time-dependent reaction theory within the Hartree-Fock framework.

G. Approximate wave functions at late times; cross sections

The TD-$\mathcal{S}$-HF method can be resummarized by statement that the Schrödinger wave function is approximated at early (precollision) times by

$$\Psi \approx \Phi_i(t) \tag{24}$$

and at late (postcollision) times by

$$\Psi \approx \sum_f \hat{\bar{\mathcal{S}}}_{fi} \Phi_f(t)\,. \tag{25}$$

Equations (24) and (25) constitute a complete and unambiguous specification of the reaction process initiated in channel $\{i\}$: the probability that one measures the system to have the properties of channel $\{f\}$ at times long after the collision is given by

$$P_i(\{f\}) = |\hat{\bar{\mathcal{S}}}_{fi}|^2\,. \tag{26}$$

Because of the fact that nuclear reaction experiments are conducted with nearly continuous beams of particles rather than with isolated single particles, such as this theory describes, their results are customarily expressed in terms of differential cross sections, rather than as probabilities (26). To relate $\mathcal{S}_{fi}$ to a cross section we must assume that the initial particles are delivered towards the target at a constant density per unit area and per unit time and calculate the arrival rate of particles (f) at some distant macroscopic counter intercepting a solid angle $d\Omega$ at angle Ω with respect to the beam. Thus both initial and final impact parameters become unspecified and one must average the probabilities over initial impact parameters and sum them over final parameters to obtain the differential cross section. The result is

$$\frac{d^n\sigma_{(i)\to(f)}}{d^{n-1}p_{(f)}d\Omega_{(f)}}=\iint dA_i\iint dA_f\,|\hat{\bar{\mathcal{S}}}_{fi}|^2\Big/\iint dA_i\,, \tag{27}$$

where the element of surface area dA_c lies in the plane perpendicular to their mean relative channel velocity $\vec{v}_c^{\,\mathrm{Rel}}$ and is given in terms of the channel impact parameter b_c and its azimuthal angle ϕ_c as follows:

$$dA_c=b_c\,db_c\,d\phi_c\,. \tag{28}$$

In Eq. (27), (i) and (f) constitute the complete set of labels [cf. $\{i\}$ and $\{f\}$ of Sec. VI, Eq. (30)] for the respective channels, except only for the impact parameters, which are well defined, for fixed $(\vec{v}_f^{(1)},\vec{v}_f^{(2)})$, by $\vec{R}_f/|\vec{R}_f|$. Also, the cross section (27) is written as the microscopic differential cross section in which each of the complete set of channel parameters $p_{(f)}$ in (f) is presumed to have been measured. In practice, most of these parameters will also be summed and/or integrated over to correspond to the less than total measurement of final state characteristics of most experiments.

H. Generality of $\hat{\bar{\mathcal{S}}}$ prescription

Note that the prescription (21) for $\hat{\bar{\mathcal{S}}}_{fi}$ might be applied independent of the particulars of the time evolution operations $U^{(\pm)}$ in Eqs. (16) and (17). It presents therefore a generally applicable alternative to the use of the initial-value solution Φ_i in Eq. (16), alone, not just for the Hartree-Fock problem, but for any approximate description of the time evolution of a reaction process by means of a wave function to which the statistical interpretation of quantum mechanics, Eq. (22), is expected to apply. In Sec. VIII below we suggest that Axiom II, Eq. (22), is plausibly necessary for interpreting *any* alleged wave function physically. For without some such assumption, one is in difficulty to argue that the quantities Φ are Schrödinger "wave functions" in any operational sense.

I. Summary of TD-$\mathcal{S}$-HF

We note the following features of TD-$\mathcal{S}$-HF:

(1) The once-only calculation of the late-time values of $\Phi_i^{(+)}(t)$, the multi-outgoing channel TDHF wave function of the conventional TDHF, is augmented by one additional calculation (backwards in time) of $\Phi_f^{(-)}(t)$ *for each final channel.*

(2) A time average of the overlap

$$\langle\Phi_f^{(-)}|\Phi_i^{(+)}\rangle=\mathcal{S}_{fi}(t) \tag{29}$$

yields the (unnormalized) $\bar{\mathcal{S}}_{fi}$, and normalization yields $\hat{\bar{\mathcal{S}}}_{fi}$, the S-matrix analog.

(3) By the choice of the averaging interval, *no* post-breakup *spurious cross channel correlations* enter into $\hat{\bar{\mathcal{S}}}_{fi}$ from either Φ_i or Φ_f. Separated configurations are propagated only by single channel self-consistent Hartree-Fock Hamiltonians.

J. Qualitative features of TD-$\mathcal{S}$-HF: Focus on definition of channels

It is remarkable that this reformulation of the TDHF description for multichannel processes is able still to conform to the requirement that each wave function at each moment be described as a single determinant, evolving self-consistently by TDHF, and that at the same time it can obviate the post-breakup spurious cross channel correlations within a single-determinantal description of a multichannel physical situation—the ravages of which appear inescapable in the straightforward time integration of the TDHF equation from the initial incoming state to a post-breakup time. Since here a calculation backwards in time is used to propagate each of the final configurations through the asymptotic region backwards into the interaction region by means of a single channel determinant, such spurious cross channel correlations never enter in the description of well-separated fragments.

In addition, the new theory exhibits a structure symmetric in time, which corresponds well with the S-matrix formulation of the exact scattering theory and provides a framework which *requires* for both initial and final states precise labels which are appropriate for the elementary objects which the scattering process describes. In contrast, the conventional initial-value TDHF method, in which only the (nearly unique) initial state needs to be constructed, allows one to overlook the need for a precise specification of labels required to characterize the asymptotic states.

We turn in Sec. VI to a consideration of what these channel labels should comprise, and obtain therefrom a statement of what a channel in the TD-$\mathcal{S}$-HF description is to specify. The sought-after result is a clear and concise definition of the *physical range* of TD-$\mathcal{S}$-HF. The answer is that the TD-$\mathcal{S}$-HF theory describes the reactions of TDHF droplets; the mathematical substance of that answer lies in the (well-defined) mathematical properties of such TDHF droplets. We find, however, one still open qualitative dichotomy in the theory—whether the TDHF droplets are classical or quantized—which the system itself must resolve according to the still unknown properties of its periodic solutions. The technical implications of that resolution are discussed further in Sec. VII.

VI. IMPLICATIONS OF $\mathcal{S}$-MATRIX STRUCTURE FOR TIME-DEPENDENT HARTREE-FOCK REACTION THEORY

By its very structure, the $\mathcal{S}$-matrix reformulation of the time-dependent Hartree-Fock theory forces the notion of reaction channels into a position of special prominence. In this section we consider what choices for these channels might be appropriate. We require that an acceptable choice should be mathematically consistent, and physically specific within the limits of the approximation, and unambiguous in both respects.

A. Initialization and asymptoticity requirements for asymptotic channels

Thus the channel labels must be sufficient (A) to initialize the Hartree-Fock propagation towards the collision, and (B) to characterize an exhaustive set of measurements upon the far separated fragments, the results of which must be independent of the distance of the (distant) measuring apparatus from the collision volume. We refer to condition (A) as the "initialization" requirement and (B) as the "asymptoticity" requirement.

In Schrödinger theory, condition (A) is guaranteed by the mathematical structure of the equation and the sufficiency of the initial wave function to determine a unique solution.[32] Condition (B), on the other hand, is fulfilled because there exists a time-independent asymptotic Hamiltonian describing a complete set of eigenstates for every possible set of fragments, and because the linearity of the equation allows the superposition of these channel eigenstates to specify *any* exact solution in terms of unique, asymptotically time-independent amplitudes, each directly related to a specific reaction channel. Conversely, it allows *any* exact solution to be (uniquely) decomposed into a linear combination of such asymptotic channel eigenstates.

B. Nonlinearity of TDHF precludes linear combination of solutions

In contrast, for the single-determinantal Hartree-Fock theory, the dynamical evolution is described not by a linear time-independent Hamiltonian but by the nonlinear time-dependent Hartree-Fock Hamiltonian. Thus, a sum of solutions is generally not itself a solution. Nor is there any guarantee that the Hamiltonian will become time independent, even at asymptotically great separations. Thus one lacks here the very basis for selecting physical asymptotic channel solutions which makes this choice so natural and obvious in the Schrödinger theory. Also lacking is the possibility of combining such solutions to build the full time-dependent solution, for such a sum can here not be guaranteed to be itself a solution nor, even, a single determinant.

C. No automatic choice of channels

Within the TDHF framework, therefore, the choice of channel characteristics is in no way an automatic process. Indeed, we utilize it as the means for testing the very consistency of the Hartree-Fock axiom with the physical requirements for a reaction theory. We therefore set out purposely to find channel labels which honor initializability and which at the same time guarantee asymptoticity for the theory.

To this purpose we should have liked to require that an acceptable channel label f specify

(i) completely, two well-separated subdeterminants (which therefore guarantee an integral number of nucleons[72] in each fragment) at some (arbitrary) large standard separation distance R_s at the time t_f;

(ii) the subdeterminants so specified translate in time and space under TDHF propagation *without change* of their internal properties.

Such conditions would define asymptotic states adequate to initialize [in accordance with (A)] specific solutions of TDHF for separate fragments. Moreover, by condition (ii) these fragments propagate towards or away from one another without change, thereby honoring the asymptoticity requirement (B) of a reaction theory.

D. Periodic solutions meet weak asymptoticity condition

Condition (ii) is surely satisfied by the translating stationary solutions of the TDHF problem for the isolated droplets. For if the wave function is stationary, then certainly all the properties it describes remain constant in time. But a less stringent interpretation of requirement (ii) allows also translating, periodically oscillating solutions as adequate channel functions for the separate TDHF droplets. Then all the properties of the droplet state, defined as time averages over the period of the drop, would propagate unchanged, in a weaker, but perhaps adequate, analogy with the eigenvalues of the channel eigenfunctions of the exact Schrödinger theory, whose instantaneous constant values are, of course, equal to their time-averaged values.

Pending further development of our knowledge of the periodic and stationary states of the TDHF problem, we adopt this more inclusive choice and consider the "periodic" solutions[29] of the isolated TDHF droplet (including the stationary states, which we consider to be periodic with period zero) as the appropriate states from which to construct the asymptotic channel wave functions of the TDHF theory.

E. Time averaging again enters naturally with periodic solutions

We note that once again, from considerations apparently independent of those which required the time averaging of $\mathcal{S}_{fi}(t)$, we are lead also to time averaging as a natural process for interpreting the single-determinantal theory. In Sec. VII, we shall see that in still a third aspect of the problem, the time-averaged interpretation may restore to the theory an adequate practical facsimile of the channel orthogonality property which, although automatic in the exact linear theory, is missing from the single-determinantal theory. Thus one can reasonably begin to entertain the suspicion that the time-averaged interpretation is not merely a convenient device, but perhaps a fundamental feature of the physical content of TDHF. Specifically, we show that time averaging allows the restoration of a form of orthogonality essential to the physical interpretation (22), and alleviates thereby some of the mathematical awkwardness which follows from the state-dependent nonlinearity of $\mathcal{H}_{\mathrm{HF}}$. Although it does not thereby retrieve the Fourier transform as a guaranteed mechanism for transforming from the time-dependent description to the description in terms of stationary (and orthogonal) eigenstates, it at least allows the consistent formulation of a single-determinantal theory which is structurally analogous to the time-dependent Schrödinger theory.

F. Specific labeling of initializable, asymptotic channels

We thus arrive at the following prescription for a suitable TD-$\mathcal{S}$-HF reaction channel: A channel is prescribed by these labels sufficient to initiate a time-dependent Hartree-Fock solution which propagates in time at large separation so as to describe (a) the translation of a well-defined target and a well-defined projectile towards one another (e.g., in the center of mass frame) and (b) periodic (including the stationary states[73] of period zero) oscillations of the internal wave functions of the fragments, whose time-averaged expectation values define the physical content of the channel states.

Then the following labels suffice to define the channel $\{f\}$:

$$\{f\} = \{(A_f^{(1)}, \lambda_f^{(1)}, \vec{v}_f^{(1)}); (A_f^{(2)}, \lambda_f^{(2)}, \vec{v}_f^{(2)}); \vec{R}_f/|\vec{R}_f|, t_f\}. \tag{30}$$

This set of labels specifies two well-separated determinants. The first determinant $(A_f^{(1)}, \lambda_f^{(1)}, \vec{v}_f^{(1)})$ describes $A_f^{(1)}$ nucleons ($N_f^{(1)}$ neutrons and $Z_f^{(1)}$ protons) in a periodic TDHF state, $\lambda_f^{(1)}$ (characterized perhaps by several real numbers), translating with velocity $\vec{v}_f^{(1)}$; likewise, for the set $(A_f^{(2)}, \lambda_f^{(2)}, \vec{v}_f^{(2)})$. We assume that all TDHF calculations are initiated at the same large standard separation distance $|\vec{R}_f| = R_s$. The label $\vec{R}_f/|\vec{R}_f|$ then defines the initial spatial locations of the two fragments, and t_f denotes the time at which the calculation is initiated.

G. Center of mass frame and orbital angular momentum

We work always in the center of mass frame so that $\vec{v}^{(1)}$ and $\vec{v}^{(2)}$ are related by the zero-momentum condition

$$A_f^{(1)}\vec{v}_f^{(1)} + A_f^{(2)}\vec{v}_f^{(2)} \equiv 0 \tag{31a}$$

and therefore together involve only one independent three-vector, say, $\vec{v}_f^{(1)}$. The separation vector $\vec{R}_f$ and their relative velocity defines their relative angular momentum $\vec{L}_f$. $\vec{R}_f$ is related to the initial positions $\vec{R}_f^{(1)}$ and $\vec{R}_f^{(2)}$ of the fragments by

$$\vec{R}_f^{(1)} - \vec{R}_f^{(2)} = \vec{R}_f\,, \tag{31b}$$

and by the center of mass condition,

$$\vec{R}_f^{(1)}A_1 + \vec{R}_f^{(2)}A_2 = 0\,. \tag{31c}$$

Also, the orbital angular momentum $\vec{L}_f$ is given explicitly by

$$\vec{L}_f = MA_f^{(1)}(1 + A_f^{(1)}/A_f^{(2)})(\vec{R}_f^{(1)} \times \vec{v}_f^{(1)})\,. \tag{32}$$

H. Determinant as product of subdeterminants

The initializing wave function for this set of labels is constructed at time $t = t_f$ as a single $(A_1 + A_2) \times (A_1 + A_2)$ determinant formed by antisymmetrizing the product of an $(A_1 \times A_1)$ determinant describing the isolated A_1-particle Hartree-Fock system located at time $t = t_f$, at $\vec{R}_f^{(1)}$ in the center of mass system and translating with velocity $\vec{v}_f^{(1)}$, and an analogous $(A_2 \times A_2)$ determinant centered at time $t = t_f$ at $\vec{R}_f^{(2)}$ in the center of mass system and translating at velocity $\vec{v}_f^{(2)}$:

$$\Phi_f(\vec{x}, t_f) = \mathcal{A}[\Phi_1(\vec{x}_1 - \vec{R}_f^{(1)}, \vec{v}_f^{(1)}, t_f)\Phi_2(\vec{x}_2 - \vec{R}_f^{(2)}, \vec{v}_f^{(2)}, t_f)]\,. \tag{33}$$

Here $\mathcal{A}$ denotes the antisymmetrizer, $\vec{x} = (\vec{x}_1, \vec{x}_2)$ symbolizes all of the $A_1 + A_2$ nucleonic coordinates, and the center of mass condition (31c) relates $\vec{R}_f^{(1)}$ and $\vec{R}_f^{(2)}$.

I. Translating, vibrating single-particle states

The subdeterminant Φ_1 is constructed by selecting the determinantal wave function for the desired initial instant of the periodic motion (labeled by $\lambda^{(1)}$, and then centering it at $\vec{R}_f^{(1)}$, and altering it so that it will translate with velocity $\vec{v}_f^{(1)}$ by the following replacement for each single-particle state:

$$u_j(\vec{x}_k, t_f; \lambda_f^{(1)}) \to \tilde{u}_j(\vec{x}_k, t_f; \lambda_f^{(1)}, \vec{R}_f^{(1)}, \vec{v}_f^{(1)}) = u_j(\vec{x}_k - \vec{R}_f^{(1)}, t_f; \lambda_f^{(1)}) \exp[i(M\vec{v}_f^{(1)} \cdot \vec{x}_k/\hbar)] \quad (j, k = 1, 2, \ldots, A_1)\,. \tag{34}$$

In a like manner is Φ_2 constructed.

J. Time-dependent asymptotic states

The time evolution of the wave function Φ_f in the asymptotic region is described by the TDHF equation (3). Because of the Gallilean invariance of the two-body interaction, the translating time-dependent single-particle functions (34) are given very simply in the asymptotic region in terms of the phase quasiperiodic single-particle functions,[29] $u_j(\vec{x}_k; t; \lambda^{(1)})$, as follows:

$$\tilde{u}_j[\vec{x}_k, t; \lambda_f^{(1)}, \vec{R}_f^{(1)}, \vec{v}_f^{(1)}] = u_j[\vec{x}_k - \vec{R}_f^{(1)} - \vec{v}_f^{(1)}(t - t_f), t; \lambda_f^{(1)}] \times \exp\{i[(M\vec{v}_f^{(1)} \cdot \vec{x}_k)/\hbar - tM(\vec{v}_f^{(1)})^2/2\hbar]\} \quad (j = 1, 2, \ldots, A_1)\,. \tag{35}$$

Here $\vec{x}_k$ are the coordinates of the kth particle, $u_j(\vec{x}_k, t; \lambda^{(1)})$ is given explicitly by the form

$$u_j(\vec{x}_k, t; \lambda^{(1)}) = P_j(\vec{x}_k, t; \lambda^{(1)}) \exp - \{i\langle E_\lambda^{(1)}\rangle t/\hbar A_1\}\,, \tag{36}$$

where P_j is periodic in time with period $2\pi/\omega_\lambda^{(1)}$, and $\langle E_f^{(1)}\rangle$ is the energy of the A_1 particle system vibrating in the periodic state $\lambda_f^{(1)}$, with its center of mass at rest. An equal share of the time-dependent phase associated with the translation of fragment (1) has been arbitrarily assigned in (35) to each of the single-particle states participating in the periodic vibration $\lambda_f^{(1)}$. This is of no physical import since only the total time-dependent phase of the full determinant is of physical significance.[30,31] The single-particle wave function (36) and the determinant constructed by antisymmetrizing the product of $A^{(1)}$ such functions are both "phase quasiperiodic" functions, comprising a product of a time-dependent, space-independent phase factor of one period and a space-dependent factor of a different period.

In this way the labels $\{f\}$ given by (30) suffice to initialize the calculation for channel f, and to specify the explicit time-dependence of the function in the asymptotic region. For the special case where the separated nuclei are in their stationary Hartree-Fock ground states, these labels (except for t_f, discussed below) comprise precisely the information commonly used to initiate a conventional TDHF calculation.[74]

K. Starting time an appropriate channel label for localized packet theory

The label t_f sets the clock for the starting point of the Φ_f calculation. It serves the essential role of distinguishing among final states which have identically structured fragments moving over identical final spatial trajectories, but which arrive at the separation R_s at different times. When only one Φ_i is involved (as in conventional TDHF) the value of t at the starting point is irrelevant. When two or more wave functions Φ_i, Φ_f are involved, as in (18), the difference between their starting times is essential to the unambiguous definition of $\mathcal{S}_{fi}$. The difference of the channel starting time labels t_f-t_i specifies this characteristic difference. If by convention Φ_i is always initiated at $t = 0$, then t_f for the final channel suffices to fix this property.

Although the occurrence of a channel label like t_f would seem natural enough for a discussion of the arrival of classical particles, it is not familiar from Schrödinger scattering theory. It occurs here because the TDHF theory *necessarily*[75] describes packets localized in all three spatial dimensions, whereas Schrödinger theory is usually formulated in terms of incoming stationary plane waves of infinite extent. Thus one need not be surprised that the labels here for the asymptotic trajectories of fully localized packets resemble the labels for a classical orbit theory.

L. TDHF droplets as objects of TD-$\mathcal{S}$-HF theory

In the TD-$\mathcal{S}$-HF description, the set of all the translating, periodically vibrating, A_1-particle subdeterminantal solutions, encompassed by the labels $(A_f^{(1)}, \lambda_f^{(1)}, \vec{v}_f^{(1)})$ in (30) comprises a dynamical subsystem of its own, which we label the A_1-particle TDHF droplet. The physical properties of an isolated TDHF droplet are completely prescribed by its time-dependent wave function, which in turn is specified for all time by any given initial-value determinant and its subsequent time-evolution under the time-dependent Hartree-Fock equation. We assume that these physical properties can be exhaustively characterized in terms of its periodic solutions (including the stationary solutions of period zero); that is, we assume that these states, or some subset of them, form a complete set.

Thus we come to the following succinct statement of our results so far: The $\mathcal{S}$-matrix restructuring of the TDHF theory of reactions prescribes the physical range of the theory as encompassing the collisions of these mathematically well-defined TDHF droplets.

VII. PROPERTIES OF TDHF DROPLETS AND THE TD-$\mathcal{S}$-HF CHANNELS

We have arrived at a point where the physical possibilities of the TD-$\mathcal{S}$-HF reaction theory are found to be constrained by the properties of TDHF droplets, and most especially of their periodic excitation spectrum.

A. TDHF droplets are oversimplified as nuclear models

In the first place we note that the TDHF droplet is essentially a simpler object than the nucleus. For it is completely described at time by a single-determinantal wave function which conveys[76] precisely the same physical information as the single-particle density matrix (a function in 6 space dimensions, e.g., for any number A of spinless identical Fermions), whereas the exact Schrödinger solution specifies completely the exact A-particle density matrix (a function in $6A$ space dimensions for A spinless identical Fermions). More briefly stated, the determinant omits all the spatial correlations (except those due to antisymmetrization) contained in the exact description: the two particle density matrix is a (antisymmetrized) product of one particle density matrices. It follows that the spectrum of excited states of the TDHF droplet must differ from that of the actual nucleus. And the physics of their energetic collisions must also be different in so far as it is influenced by two-particle correlations.

One thus infers that attention should be focused upon the differences between the spectra of TDHF droplets and those of nuclei as the appropriate basis for learning specifically how the determinantal approximation should be expected to fall short of the exact Schrödinger description. This problem will be addressed elsewhere in more detail.

B. Channel orthogonality and the statistical axiom

At a deeper level, we are forced by the very structure of the present theory to raise here a far move awkward question, whether there can consistently exist *any* channels which will display asymptoticity, even on the time average, under the basic statistical interpretation, Eq. (18), of the physical content of a wave amplitude?

So far we have succeeded in providing for the initialization of the calculation of final state amplitudes $\Phi_f^{(-)}$ and in guaranteeing that any one specific channel wave function preserves unchanged the (time-averaged) physical information about the internal state of the outgoing drop as it propagates away from the collision. But consistent application of the statistical interpretation requires us to inquire also about the overlaps among *different* channel wave functions in the asymptotic region. For if two channel wave functions $\{f\}$ and $\{f'\}$ exhibit a finite overlap, then application of the statistical interpretation to them requires that the finite overlap amplitude, $\Theta_{ff'}$ be interpreted as indicating a certain probability that the final state $\{f\}$ will be measured as $\{f'\}$. Thus, nonorthogonality of the asymptotic channel states implies under the statistical interpretation transitions, or at least admixtures among the various channel amplitudes, even in the asymptotic region.

Except on a time-averaged basis, such overlaps will generally be nonzero, since the periodic single-determinantal solutions exhibit in no way the general orthogonality property which adheres to the eigenfunctions of the linear Schrödinger theory. (Note that even the zero-period stationary Hartree-Fock states will in general not be mutually orthogonal.)

C. Time-averaged asymptotic channel orthogonality

But the process of time averaging is able under certain circumstances to restore a kind of mutual "orthogonality" among the reaction channels, as we now discuss. The orthogonality is defined in terms of the following time-averaged overlap between channel amplitudes:

$$\Theta_{ff'} = \lim_{\tau\to\infty}\frac{1}{2\tau}\int_{t-\tau}^{t+\tau}\langle\Phi_f^{(-)}(t')|\,\Phi_{f'}^{(-)}(t')\rangle dt' \quad (t>\tau). \tag{37}$$

Here $\lim_{\tau\to\infty}$ implies that τ in practice is to be much larger than any of the periods in $\{f\}$, $\{f'\}$, and in fact large enough so that the integral results in a constant time-averaged value for $\mathcal{O}_{ff'}$.[77] Also, t must be large enough to allow the asymptotic properties of the wave functions to be fully realized over the whole time-averaging interval. In particular, at the earliest time $t' = t - \tau$ in (37) the fragments in each channel must be well separated.

D. Implications of channel nonorthogonality

Only if $\mathcal{O}_{ff'}$ vanishes for all channels $\{f\} \neq \{f'\}$, can we realize a theory in which the probability of each of the possible final internal states of the droplet is well defined by a given reaction amplitude. Otherwise the theory describes reaction amplitudes each of which describes not the probability amplitude for one final state, but instead amplitudes for some set of nonorthogonal final states. Then every reaction amplitude contributes to every nonorthogonal final state, and the theory collapses to a description of some time-dependent *distribution* of internal final channel states defined, not only by the reaction dynamics, but also by the mutual nonorthogonalities among the asymptotic channel states. We elaborate the physical interpretation of this solution further in Secs. VII H through VII L below, discussing first the mathematical circumstances of the channel overlaps.

E. Conditions for orthogonality

We shall demonstrate that the properties of the overlaps $\mathcal{O}_{ff'}$ depend essentially upon the nature of the periodic TDHF solutions. To see this, we consider the expression (37) more explicitly, using the expressions (35) for the translating, periodic solutions.

Then we can see at once that for two channels $\{f\}$ and $\{f'\}$ labeled as in (30), the asymptotic overlap $\mathcal{O}_{ff'}$ in (37) will surely vanish (for the reason given in parenthesis) unless each and every one of the following conditions[78] is fulfilled:

(a) $A_f^{(1)} = A_{f'}^{(1)}$, and $A_f^{(2)} = A_{f'}^{(2)}$ (otherwise at least one single-particle wave function in $\{f\}$ is spatially orthogonal to one in $\{f'\}$);

(b) $\vec{v}_f^{(1)} = \vec{v}_{f'}^{(1)}$, and $\vec{v}_f^{(2)} = \vec{v}_{f'}^{(2)}$ (otherwise the overlaps can remain finite at most for a brief finite interval, and must therefore average to zero over the extended interval, 2τ);

(c) $t_f = t_{f'}$ (otherwise the localized wave packets would never occupy the same spatial location[78] at any given time);

(d) $\vec{L}_f = \vec{L}_{f'}$ (otherwise the wave packets in f, f' would asymptotically have distinct impact parameters, and a vanishing spatial overlap[78] integral);

(e) the droplet excitation energies, $E_f^{(1)}$, $E_f^{(2)}$, $E_{f'}^{(1)}$, $E_{f'}^{(2)}$, corresponding to periodic TDHF solutions are discrete and nondegenerate. (This condition is discussed in some detail below.)

We summarize the honoring of the conditions (a) through (d) by starting that the two channels $\{f\}$, $\{f'\}$ "have the same trajectory," emphasizing thereby that only condition (e) involves the internal periodic states of the channel fragments. Thus conditions (a)–(d) are to be considered kinematical while condition (e) alone involves the internal dynamics of the systems.

F. Analysis of time-averaged channel orthogonality

Indeed, condition (e) is also the pivotal condition for establishing or disestablishing the time-averaged channel orthogonality. Since $u_i(\vec{x}_j, t; \lambda_f^{(1)})$ in (34) is periodic, its time dependence can be expressed in the form

$$u_j(\vec{x}_k, t; \lambda_f^{(1)}) = \sum_q U_q^j(\vec{x}_k : \lambda_f) \exp(iq\omega_f^{(1)} t) \quad (q \text{ integral}), \tag{38}$$

where the fundamental frequency

$$\omega_f^{(1)} = 2\pi / T_f^{(1)} \tag{39}$$

is defined by the period $T_f^{(1)}$ of the vibration $\lambda_f^{(1)}$. Then the full time-dependence of the integrand of $\mathcal{O}_{ff'}$ in (37) is obtained from (38) and (36):

$$\mathcal{O}_{ff'} = \lim_{\tau\to\infty} \sum_{S_f, S_{f'}} (2\tau)^{-1} \int_{t-\tau}^{t+\tau} dt' I(S_f, S_{f'}) \times \exp\{i[(E_f' - E_f)/\hbar + \Delta_{ff'}]t'\}. \tag{40}$$

Here E_f (or $E_{f'}$) is the total energy of channel f [or (f')],

$$E_f = A^{(1)} M \vec{v}_f^{(1)2}/2 + A^{(2)} M \vec{v}_f^{(2)2}/2 + E_f^{(1)} + E_f^{(1)} + E_f^{(2)}; \tag{41}$$

$\Delta_{ff'}$ is given by

$$\Delta_{ff'} = S_{f'}^{(1)} \omega_{f'}^{(1)} + S_{f'}^{(2)} \omega_{f'}^{(2)} - S_f^{(1)} \omega_f^{(1)} - S_f^{(2)} \omega_f^{(2)}. \tag{42}$$

Here $S_f = (S_f^{(1)}, S_f^{(2)})$, and $S_{f'} = (S_{f'}^{(1)}, S_{f'}^{(2)})$ are pairs of integral sums of integers q, and $I(S_f, S_{f'})$ is a sum of spatial integrals, constant in time. Thus the time integration in $\mathcal{O}_{ff'}$ reduces it to the form

$$\mathcal{O}_{ff'} = \lim_{\tau\to\infty} \sum_{S_f, S_{f'}} (2\tau)^{-1} I(S_f, S_{f'}) 2 e^{i z_{ff'} t} (\sin z_{ff'}\tau)/z_{ff'}, \tag{43}$$

where

$$z_{ff'} = \{(E_f - E_{f'})/\hbar + \Delta_{ff'}\}\,, \tag{44}$$

and like $\Delta_{ff'}$, is a function of $S_f, S_{f'}$.

We next show that $\Theta_{ff'}$ is, for discrete vibrational energies, $E_f^{(1)}$, $E_f^{(2)}$, a singular function of $\{f\}$, $\{f'\}$ equal to one for $\{f\}=\{f'\}$, zero otherwise.

Consider first the case $\{f\}=\{f'\}$. Then in the definition (37) of $\Theta_{ff'}$ one can employ the normalization condition on the wave functions,

$$\langle\Phi_f(t')|\,\Phi_f(t')\rangle = 1 \tag{45}$$

to obtain immediately

$$\Theta_{ff} = \lim_{\tau\to\infty}(2\tau)^{-1}\int_{t-\tau}^{t+\tau} dt' = 1\,. \tag{46}$$

This result can also be obtained by manipulation of (43). Then, since for $\{f\}=\{f'\}$

$$z_{ff} \equiv 0\,, \tag{47}$$

one finds

$$\lim_{\tau\to\infty}\tau z_{ff} = 0\,, \tag{48}$$

and (43) reduces again to the normalization integral

$$\Theta_{ff} = \sum_{S_f} I(S_f, S_f) = 1\,. \tag{49}$$

For $\{f\}\neq\{f'\}$, $\Theta_{ff'}$ is already known by Sec. VII E to vanish when the trajectories differ. For channels $\{f\}\neq\{f'\}$ with the same trajectory one finds (according to the discussion of Sec. VII G, below) that

$$z_{ff'} \neq 0\,, \tag{50}$$

if the energy spectrum of the periodic vibrations is discrete. Therefore, in this case one obtains instead of (48), the result

$$\lim_{\tau\to\infty}\tau z_{ff'} = \infty \tag{51}$$

and (43) reduces to the value zero, as follows:

$$\Theta_{ff'} = \lim_{\tau\to\infty}\sum_{S_f, S_{f'}} (2\tau)^{-1} I(S_f, S_{f'})\, 2e^{iz_{ff'}t} \times (\sin z_{ff'}\tau)/z_{ff'} \tag{52a}$$

$$= \sum_{S_f, S_{f'}} I(S_f, S_{f'})\, e^{iz_{ff'}t} \lim_{\tau\to\infty}\{(\sin z_{ff'}\tau)/z_{ff'}\tau\} \tag{52b}$$

$$= 0\,, \{f\}\neq\{f'\}\,. \tag{53}$$

Equation (53) establishes the time-averaged "orthogonality" of pairs of channels with $z_{ff'} \neq 0$.

G. Discrete energy spectrum is crucial to orthogonality

We now show that the condition (50) is equivalent for channels with the same trajectory [conditions (a)–(d) of Sec. VII E, above] (apart from accidental degeneracies, to be defined more precisely below) with the condition that the internal channel energies be discrete.

Consider the quantity $\Delta_{ff'}$ defined in Eq. (42). For summands in (43) for which $\Delta_{ff'}$ vanishes, $z_{ff'}$ vanishes, $z_{ff'}$ defined by (44) can vanish if and only if[79]

$$E_f^{(1)} + E_f^{(2)} = E_{f'}^{(1)} + E_{f'}^{(2)}\,. \tag{54}$$

[When the trajectories f, f' are the same, the kinetic energies in (41) cancel in (44), leaving here only the internal energies.] If the vibrational energy spectrum is descrete then (54) can be honored only if two unrelated discrete real numbers happen to be equal. But if the spectrum is continuous, then equality will always prevail for some properly chosen vibrations λ_f and $\lambda_{f'}$.

Equalities between unrelated discretely valued real numbers, such as required by Eq. (54) and Eq. (55) below, comprise a subset of measure zero of the set of pairs of real numbers. We therefore refer to such equalities as "accidental degeneracies," and assume in this treatment of the theory that they do not occur. When they occur, they shall require special treatment not considered here.

Thus it follows that if the spectrum of periodic vibrations is discrete (54) cannot in general be satisfied, and condition (50) prevails.

If for some summand(s) of (43) $\Delta_{ff'}$ does not vanish then $z_{ff'}$ can vanish if and only if

$$E_f^{(1)} + E_f^{(2)} - E_{f'}^{(1)} - E_{f'}^{(2)} = S_f^{(1)}\hbar\omega_f^{(1)} + S_f^{(2)}\hbar\omega_f^{(2)} - S_{f'}^{(1)}\hbar\omega_{f'}^{(1)} - S_{f'}^{(2)}\hbar\omega_{f'}^{(2)}\,. \tag{55}$$

But since S_f and $S_{f'}$ are integers, and since the frequencies ω_f and $\omega_{f'}$ comprise a discrete set fixed by the periodic solutions for the TDHF droplet, the right-hand side of Eq. (55) can assume only numerical values from a discrete set. But the left-hand side, $E_f^{(1)} + E_f^{(2)} - E_{f'}^{(1)} - E_{f'}^{(2)}$, can exhibit a discrete or a continuous set of values, depending upon whether the periodic vibrational energies of the TDHF droplets exhibit a discrete or a continuous spectrum.

For a discrete periodic energy spectrum, the left-hand side can have only a discrete set of values. Then (55) can again be satisfied only by an equality between two unrelated discrete numbers, i.e., by an accidental degeneracy of the type assumed here not to occur. But if the energy spectrum of periodic states is continuous,[89-91] the left-hand side may exhibit a continuous range of values, and a proper selection of the pairs of droplet vibrations can always be made so that (55) is satisfied.

Thus we conclude that, apart from accidental numerical degeneracies, the quantity $z_{ff'}$ can vanish for different channels of the same trajectory if and only if the vibrational energy spectrum is continuous. There follows the result stated in Sec. VII F that asymptotic channel wave functions will, or will not, display the (time-averaged) orthogonality property (53), according to whether the energy spectrum of the periodic TDHF droplet vibrations is discrete or is continuous.

H. Statistical interpretation applied to classical TDHF droplets

If it is generally possible to meet condition (55), as when the periodic spectrum is continuous, we conclude that it is *impossible* to guarantee the mutual orthogonality (53) of different asymptotic channel functions with the same trajectory, even on the time average.

Such is the situation which prevails if one considers the small amplitude harmonic TDHF vibrations to be characteristic[80] periodic solutions of TDHF. For they allow any vibrational energy to be specified (by simple adjustment of the amplitude of vibration) for any one of the discrete infinity of "normal mode" vibrations, guaranteeing thereby that (55) is satisfied for a discrete infinity of channel pairs for every possible trajectory. We refer to such TDHF droplets, whose periodic vibrations occur at continuous values of the energy as "classical" TDHF droplets.

In the case of such classical TDHF droplets, the consistent application of the statistical interpretation requires us to interpret our channel states, even at large separations, as continuing to make transitions among themselves. Then we conclude that the reaction amplitudes of the theory, describe not just the dynamical effects of the interaction in exciting specific excited states of the TDHF droplet, but also a postreaction equilibrization process inherent in the droplet itself which continues to occur even after the interaction has ended, and in which each droplet continues, even in the asymptotic region, to share its internal energy among its energy-degenerate periodic vibrations. Such a process might ultimately lead either to some specific "equilibrium" or thermalized distribution among the vibrations, or it might lead to a droplet roaming endlessly in time through the available phase space.

The physical implication for the TD-$\mathcal{S}$-HF reaction theory description of these classical TDHF droplets is qualitative: As a matter of principle, no measurable result can be consistently predicted from the theory which is independent of the (distant) position of the measurement apparatus, except those which involve constants of the motion in the asymptotic trajectories, such as

(a) the mass of each fragment $A^{(1)}, A^{(2)}$;

(b) the asymptotic center of mass momentum of each of the two fragments $A^{(1)}\vec{v}^{(1)}$, $A^{(2)}\vec{v}^{(2)}$;

(c) the orbital angular momentum $\vec{L}$ of Eq. (32);

(d) the average vibrational energy of each fragment, $E^{(1)}$, $E^{(2)}$;

(e) other constants of the TDHF solution of the separate fragments, such as the one-body operators which commute with the exact Hamiltonian (as discussed in the Appendix).

In particular, no more specific information about the internal states of the emerging droplets can be specified as an asymptotically time-independent property of the reaction process.

Then the TD-$\mathcal{S}$-HF reaction theory is reduced to a "trajectory theory" since its own internal structure would preclude consistent prediction of physical measurements other than the trajectory characteristics, (a), (b), (c), (d), and (e). In particular, no characteristics unique to a specific periodic final excited state could be predicted. This is in sharp contrast to the quantal Schrödinger theory which allows in principle an exhaustive set of quantum numbers to be measured for each final channel eigenstate.

I. Classical TDHF droplets are intrinsically dissipative

This property, we summarize by the statement that the classical TDHF droplets are "intrinsically dissipative." As a direct consequence of the fact that they exhibit a continuous energy spectrum for their periodic motions, they exhibit *at every energy* at least a discrete infinity of degenerate states, which states in general are not orthogonal, and therefore cannot escape, under consistent application of the statistical interpretation, the implication of perpetual intertransitions. Thus at *every* energy the physical properties they predict would be properties not of any specific periodic solution, but rather of the whole set of periodic solutions not asymptotically orthogonal to it. For this reason as outgoing reaction fragments they are capable of propagating asymptotically without change only those results of the reaction process associated with quantities conserved in the asymptotic region: their mass, momentum, angular momentum, energy, etc.

J. Classical droplets allow only trajectory theories

In short, we conclude that classical TDHF droplets allow an asymptotic collision theory which describes only some "equilibrized" distribution of (or worse, some chaotically wandering) internal states. Then the specific content of the theory lies solely in the distribution of the outgoing trajectories which the TDHF process generates from each given incoming trajectory. Such a limited theory would seem to fall far short of the expectations originally entertained for the single-determinantal approximation, in that nearly all of the structure for final states which its explicit many-body treatment promised is reduced, in the end, only to statements about the kinematical features of the separating droplets and their relative motion. Thus, the many-body dynamics which seemed to justify the complications of the calculations is dessicated into a result hardly commensurable[59] with the elaborate machinery which generated it. One should note that, so far, no numerical TDHF experiment has been specifically interpreted for implications other than those relating to the trajectories.

K. Classical TDHF droplets qualitatively resemble viscous classical liquid drops

We note that the properties of classical TDHF droplets, devastating as they may be to the hope for a Schrödinger-type structure in the TDHF reaction theory, are not qualitatively alien to classical physics. Indeed water droplets emerging from a collision will yield to measurement results which surely vary with time after the collision[81-85]: their own internal viscosity continually redistributes their energy irreversibly into the droplet's microscopic degrees of freedom until thermal equilibrium is attained. Thus at very great distances, water droplets also retain only that memory of the collision process which is characterized by constants of the asymptotic motion. Thus collisions of classical droplets surely lack the asymptoticity property which we have required (in Sec. VI A) of the TD-$\mathcal{S}$-HF theory. Then if TDHF droplets were found always to be classical, and no consistent requantization axiom can be found applicable (see Sec. VII N, below), then one would be forced to conclude that the single-determinantal assumption does necessarily convert the Schrödinger reaction theory into a classical theory, and indeed a classical theory of intrinsically dissipative droplets. Such a clear and specific qualitative conclusion is therefore a prospective reward of careful study of the nature of the periodic TDHF solutions.

L. Classical TDHF droplets not suitable for TD-$\mathcal{S}$-HF description

In spite of the channel nonorthogonality, one might suggest that the TD-$\mathcal{S}$-HF theory of classical droplets ought to be applied, and its predictions about physical operators interpreted as average characteristics of the whole distribution of final channels. An analogous view has in fact been adopted to resolve the interpretational dilemma of the late-time solutions to the conventional initial-value TDHF theory.

Unfortunately, the TD-$\mathcal{S}$-HF theory is too rigid axiomatically to encompass such an interpretation. For consistency with its statistical interpretation (Axiom II of Sec. V E) would require it to be recast to describe among the channels transition amplitudes analogous to those described by $\mathcal{S}_{fi}(t)$ in Eq. (18), but now occurring even at asymptotically late times when the fragments are already well separated, and to describe the subsequent time evolution of the resulting states according to (the TDHF) Axiom I. Such an alteration might in fact be possible. But, the same consistent application of the statistical interpretation requires also a recasting of the backward time-evolution process of the solutions $\Phi_f^{(-)}(t)$ for final state channels with excited internal states of the droplets at $t=t_f$. There the physical consequences are more immediately evident: the TDHF droplets must, by the time they collide, have been allowed to evolve arbitrarily far from the specified initial state, presumably into a state bearing no specific relationship to the initial state, except for its constants of the motion. Thus the physical content of the initializability property (Sec. VI A) of the channel states, as well as that of the asymptoticity property, must be altered by the reinterpretation which channel nonorthogonality requires. The resulting theory would be, again, a trajectory theory only, but one to which the whole TD-$\mathcal{S}$-HF machinery remains irrelevantly appendaged.

We conclude therefore that the TD-$\mathcal{S}$-HF theory as structured here under Axioms I and II offers no promising framework for describing properties of the reactions of classical TDHF droplets beyond their trajectory characteristics. For such cases a more appropriate theory would be specifically tailored to describe not initial and final states, but initial and final equilibrium distributions not necessarily in one-to-one correspondence with asymptotic single-determinantal wave functions. The possibility exists that such a simplified theory would be extracted from the TD-$\mathcal{S}$-HF framework by invoking a suitable average over asymptotic channels to restrict the range of the theory only to the trajectory properties, and by replacing the specific initialization process of TDHF by some suitable averaging.

M. Quantized TDHF droplets exhibit structure fully analogous to exact theory

We now consider the case when the TDHF periodic vibrational energy spectrum is discrete,[89-91] so that the crucial energy equality (55), can not generally be satisfied. For such "quantized" TDHF droplets TD-$\mathcal{S}$-HF theory obtains immediate applicability, since then the asymptotic channel overlap $\mathcal{O}_{ff'}$ (37) vanishes identically for *every* pair of channels.[86] Then the use of Axiom II for the channel wave functions $\Phi_{\{f\}}$ is fully consistent with the statement that the squared $\mathcal{S}$-matrix element,

$$|\hat{\mathcal{S}}_{fi}|^2 = P_f(i) \tag{56}$$

is to be interpreted as the probability that for a reaction initiated in channel $\{i\}$ time-averaged measurements in the asymptotic region yield the properties of channel $\{f\}$.

In this case, the TD-$\mathcal{S}$-HF theory describes transitions into a set of channels, separately characterized, for each given trajectory, by every distinct periodic solution of target and/or projectile. Such a description is fully analogous structurally to the exact Schrödinger theory; the periodic solutions of TDHF here play the role of the channel eigenstates of the Schrödinger theory.

We have already noted in Sec. VII H that a discrete periodic spectrum is not the natural extrapolation of the well-known small amplitude approximate solutions of TDHF, which are harmonic for a continuous range of small amplitudes and energies.[80] However, the existence of these approximate harmonic solutions does not preclude the possibility that the periodic states are discrete, since the small amplitude solutions are *approximate* solutions, which may in fact not satisfy rigorously the periodicity requirement for a function of period T

$$\psi(t+T)=\psi(t) \quad (\text{all } t)\,. \tag{57}$$

Indeed, it might turn out that only at certain discrete amplitudes, do these small amplitude solutions satisfy (57) exactly. Then a discrete spectrum of truly periodic states would be embedded in the continuous family of small amplitude approximately harmonic TDHF solutions, without contradiction.

Clearly, some rigorous results about the periodic TDHF solutions are an urgent prerequisite for assessing the physical possibilities of the single-determinantal theory.

N. Requantization of classical droplets: A possible future approach

We have concluded in the previous discussion that a classical TDHF droplet, whose periodic spectrum is continuous in energy, is an intrinsically dissipative object, not amenable to description by the TD-$\mathcal{S}$-HF method. Perhaps, as we suggested in Sec. VII L above, some modified theory could be extracted from TD-$\mathcal{S}$-HF to describe such classical objects.

On the other hand, we surely must expect that for energies of the order of $\hbar\omega$, where $T=2\pi/\omega$ is the period of a normal mode of the classical TDHF droplet, the energy ought on general physical grounds, to be quantized. In such a realm, we might then be forced to question the relevance of such a classical TDHF theory to the solutions of the underlying exact Schrödinger problem.

One might in fact be led to consider "requantizing" the TDHF theory of the classical droplet by adding to the theory an additional axiom which requires that for specifying asymptotic states, only those self-consistent vibrations of the TDHF system are to be allowed which have certain specific, discrete amplitudes. Then the energies allowed for such vibrating requantized TDHF droplets would also be rendered discrete.[89-91] Such a restriction, which limits channels to such requantized TDHF droplet states would qualitatively alter the results obtained for classical TDHF droplets in Sec. VII H–VII L, into the structure which prevails when the periodic solutions are of themselves discrete with "quantized" energies. For in this case, the asymptotic channels are defined by the labels of Eq. (30), but now subject to the additional condition that only those certain discrete values of the vibrational amplitudes are now allowed, corresponding to discrete energies $E^{(1)}$, $E^{(2)}$ for the droplets. Then the time-averaged overlap, $\mathcal{O}_{ff'}$ of (37) will again be guaranteed to vanish by the effect of the discrete energy spectrum requirement (55), and consequently the spontaneous transitions among channels implied by Axiom II will vanish on the time average.

For such requantized droplets, the TD-$\mathcal{S}$-HF method leads consistently to a theoretical description in which transitions occur during the collision interval to final states which propagate unchanged to large distances. Therefore, the theory once again exhibits a structure fully analogous with the exact Schrödinger quantum scattering theory.

Thus, if further study of the mathematics of the TDHF equations were to reveal that each family of periodic solutions exists for a continuous range of energies and amplitudes, then the merit of such a requantization axiom, as a means to restore to the single-determinantal theory the maximal structure of the exact theory, ought to be considered.

Needless to say, a basic question concerning such a requantization axiom would be its mutual consistency with the TDHF evolution Axiom I and with the statistical interpretation Axiom II of the present theory. We have at present no comment on that question.

Thus, at present, the requantization of the TDHF droplets is merely a possible future escape from the serious restriction the theory must suffer if the TDHF droplets, by virtue of their own periodic spectrum, do prove to be classical. The question whether they are or are not classical of and by themselves remains, of course, the question of the highest priority.[89-91]

VIII. THE STATISTICAL INTERPRETATION IN TD-$\mathcal{S}$-HF

At the center of the TD-$\mathcal{S}$-HF restructuring of conventional TDHF reaction theory lies the assumption Axiom II that the statistical interpretation must be applied to the amplitudes (18) between solutions propagated from acceptable asymptotic channel states. We discuss first of all the reasons why some form of statistical interpretation seems necessary. Later we consider from a structural viewpoint the sources of the difficulties which lead us to restrict the single-determinantal solutions considered acceptable in the TD-$\mathcal{S}$-HF theory, and thereby the range of application of the statistical assumption.

The heretofore generally accepted alternative to the application of the statistical interpretation Axiom II among the many wave functions which satisfy TDHF Axiom I, is to rule out the question. This alternative is implicitly embodied in the closed[87] conventional initial value formulation which allows, in the description of a dynamical system specified by initial conditions $\{i\}$, only the calculation of the single solution $\Phi_i(t)$. Then only time-dependent expectation values defined by $\Phi_i(t)$ are given physical significance, and expansions in terms of other functions within the theory do not arise.

We have already outlined in Sec. IV some mechanistic reasons why the conventional initial-value formulation promises to be inadequate for reaction processes. Besides these mechanistic considerations, a one-wave-function theory in which only expectation values can be computed is structurally but a pale replica of the many-body quantum scattering theory which TDHF attempts, at substantial practical cost, to model. The very fact that in its restructured TD-$\mathcal{S}$-HF form the single-determinantal theory can encompass quantum transition amplitudes among a wide variety of wave functions while still describing each channel self-consistently, still remaining entirely within the single-determinantal framework, and still admitting the statistical interpretation as a basis to construct and analyze reaction amplitudes among the wave amplitudes of the theory, is in itself a remarkable circumstance, which at least recommends caution against premature acceptance of too narrow limits for the single-determinantal theory.

Finally, the statistical interpretation seems especially appropriate for dealing with a quantity naturally expected by its source and substance to be a Schrödinger amplitude (albeit an approximate one), that its operation in some form or another appears to be intrinsically cogent. Any reasonable method for adding it, therefore, to a model which excludes it would deserve fair consideration.

Beyond the single-determinantal realm, we note that there does exist for every physical system a complete set of stationary eigenstates of the exact Hamiltonian, in terms of which any approximate wave function may be expanded. Even more, one would normally expect such an expansion to be an essential tool in the process of comparing some approximate wave function with the exact solution which it is supposed to approximate. Therefore, to *exclude* such an expansion, and the consequent statistical interpretation of its various amplitude coefficients, would necessarily preclude a comparison with the exact description one attempts by approximate methods to mimic. But to *allow any such* an expansion is to assume at least some form of statistical interpretation. For then the expansion of both Φ's in (18) yields, for a set of exact eigenstates Ψ_j:

$$\mathcal{S}_{fi}(t) = \langle \Phi_f^{(-)}(t) | \Phi_i^{(+)}(t) \rangle$$

$$= \sum_j \langle \Phi_f^{(-)}(t) | \Psi_j \rangle \langle \Psi_j | \Phi_i^{(+)}(t) \rangle \tag{58}$$

$$= \sum_j a_{fj}^{(-)}(t) a_{ji}^{(+)}(t) \tag{59}$$

as the amplitude that the state $\Phi_i^{(+)}(t)$ would be found to be $\Phi_f^{(-)}(t)$ at time t.

Thus a very persuasive support for assuming the statistical interpretation arises from the implications which must follow if it were *not true* for TDHF wave functions. For then no basis whatsoever would remain for considering *any* TDHF solution to be an approximate Schrödinger *wave function*, or even for comparing a TDHF solution with a Schrödinger solution. Then the TDHF method itself would have become *de facto* a theory for the square root of some classical probability function, but merely expressed still in the (now misleading) symbols and formalism of Schrödinger theory. In short, to *deny* the statistical assumption would seem to eviscerate the central quantum content of the single-determinantal method, and to reduce it at best to a probabilistic trajectory theory for some sort of classical droplet.

Then what of the fact that within TD-$\mathcal{S}$-HF framework only certain continuum solutions, selected on physical grounds by their asymptotic behavior, are available for applying the statistical interpretation? We view this circumstance as an inevitable result of the single-determinantal assumption of the TDHF method. For that assumption leads to a time-evolution operator $\mathcal{H}[\Phi]$ which is state dependent, and thence to a nonlinear dynamical law for the time evolution.

This nonlinearity has the practical consequence that the orthogonalizability of a linearly independent set of wave functions, guaranteed for linear theories by the possibility of carrying out a Schmidt process of linear recombination, can here not be assumed. It follows that the existence of a complete orthogonal set of solutions, to which the application of the statistical interpretation could be most naturally applied, can also not be assumed. Moreover, practical experience allows no hope that somehow orthogonality might prevail even if unguaranteed.

The TD-$\mathcal{S}$-HF theory circumvents this difficulty (cf. Sec. VI) by selecting among all possible asymptotic solutions those which describe physically acceptable reaction channels (involving periodic internal states of the TDHF droplets) and defining only those solutions which evolve from or into such asymptotic solutions to be acceptable continuum solutions of the TD-$\mathcal{S}$-HF theory.

Thus we deal here with a theory which combines fundamental qualitative elements of the exact Schrödinger theory (the statistical interpretation, the availability of a complete set of solutions, and its orthogonalizability as assured by the Schmidt application of the superposition principle) not independently, but interdependently, in such a way as to circumvent the difficulties following from the nonlinearity of the single-determinantal model problem. The process of combination consists of selecting the solutions to be included in the theory in such a way as to guarantee then the indispensable properties for a reaction theory of the Schrödinger structure, invoking the statistical interpretation among all of these selected solutions, and restricting the physical interpretation of the theory to time-averaged quantities.

The result is a model theory for time-dependent processes which has been constructed completely upon time-dependent solutions and their properties, with no reference to the complete orthogonalizable set of stationary solutions which is so useful and convenient in exact theories. Still, within the limitations which flow from its nonlinearity (which after all, is the price of the physical simplification of the exact many-body theory), the statistical interpretation is allowed its maximal range of operation and a sufficient range to retain for the model the capacity to exhibit the qualitative structure of the exact theory.

IX. POSSIBLE GENERAL APPLICABILITY TO NONLINEAR APPROXIMATE REACTION THEORIES

Besides the Hartree-Fock system, one might expect that other nonlinear approximations to the Schrödinger equation could arise. It is therefore worthwhile to emphasize that the present restructuring of the TDHF reaction theory from an initial-value problem into a theory describing transitions from initial to final states depends essentially upon the periodicity and the translational properties of the solutions of bound isolated subsystems, and is entirely independent of the specific characterization of TDHF, viz., the single-determinantal approximation.

It follows then that the present approach might prove applicable to a broad class of nonlinear approximate initial-value problems which purport to provide by a Schrödinger amplitude an approximate description of a reaction process. The following sequence of steps outlines such a possible extension:

(a) Assume that the nonlinear dynamical law propagates every wave function in the theory in time.

(b) Define asymptotic channel wave states in terms of the periodic solutions of the chosen dynamical law, thereby guaranteeing the asymptoticity and initializability requirements for reactions.

(c) Requantize, if necessary and possible, to guarantee time-averaged asymptotic channel orthogonality among the retained set.[89-91]

(d) Specify the acceptable continuum solutions of the theory to comprise only those which evolve from or into such asymptotic channel wave functions.

(e) Assume that the statistical interpretation applies for all amplitudes (18) between the acceptable states of the theory.

(f) Define the physical predictions of the theory in terms of the time averages of physical operators in the asymptotic channel states.

Such a procedure might suffice to define a time-averaged reaction theory for any nonlinear model of the time-dependent Schrödinger theory which exhibits periodic bound-state solutions and suitable translational behavior for its isolated droplets.

Its essential element is the assertion of the analogy between (perhaps selected) periodic bound-state solutions of the model problem and the stationary eigensolutions of the exact Schrödinger theory. As we see in the single-determinantal example, such an assertion can, at the price of the time averaging of all physical predictions, resolve the most difficult consequences of the nonlinearity in such a way as to preserve all the qualitative physical elements of the quantum reaction theory, and to lead therefore to a model theory whose structure is a faithful image of that of the exact theory.

X. SUMMARY AND CONCLUSIONS

The conventional TDHF initial-value problem has been restructured within the self-consistent single-determinantal subspace, to provide time-averaged transition amplitudes from initial to final asymptotic channels. The mathematical objects which such a theory can describe are well defined by the labels which physically appropriate channels can and must have. We have called them TDHF droplets. They may ultimately emerge as classical or quantized, depending upon the (still unknown) mathematical structure of the periodic TDHF solutions. For the classical droplets, an asymptotic reaction theory describes (at most) the equilibrized internal state of any reaction product and the trajectory of its center of mass. For quantized TDHF droplets, reaction channels occur corresponding to each of the discrete periodic internal states of a reaction product. Then the structure of the TD-$\mathcal{S}$-HF theory is fully analogous to that of the exact Schrödinger reaction theory, with the periodic TDHF solutions filling the role played by the channel eigenstates in the exact theory. The possibility exists that a suitable requantization axiom could consistently restore this structure, even for classical TDHF droplets.

It is argued that were statistical interpretation of Φ central to the present theory to be shown to be erroneous or irrelevant, the TDHF amplitude could no longer properly be considered a quantum amplitude. It is suggested also that the entire analysis is structurally applicable to *any* nonlinear approximant to the Schrödinger initial value problem in the continuum.

We conclude that the TD-$\mathcal{S}$-HF restructuring of the conventional TDHF theory offers a method for the calculation of the quantum probability for a particular final state channel to be found in a reaction, while still remaining within the space of single-determinantal wave functions, each of which evolves in time by self-consistent TDHF. At the same time, the restructured TD-$\mathcal{S}$-HF theory completely eliminates the unspecified measure of physical nonsense introduced by the post-breakup spurious cross channel correlations into the late-time description of the conventional initial-wave TDHF method.

In addition, the physical range of the single-determinantal approach has been clearly defined to be the physics of the TDHF droplets. It follows that the limits of relevance of TDHF numerical experiments to nuclear (or atomic) reaction processes can be illuminated by theoretical studies of the distinctions between TDHF droplets and realistic nuclei (or atoms).

Note added in proof. Subsequently, Kan *et al.*[90] recognized the gauge invariance of these periodic states as a natural requirement which leads to a discrete spectrum of "TDHF eigenstates." The consequences for the TD-$\mathcal{S}$-HF reaction theory follow the discussion of Sec. VIII M and are outlined in Ref. 91.

ACKNOWLEDGMENTS

The authors are indebted to many colleagues for innumerable conversations and suggestions over the extended period of this research, but especially to Dr. D. J. Rowe, Dr. T. Tamura, Dr. K.-K. Kan, Dr. M. K. Banerjee, Dr. H. Schultheis, Dr. R. Schultheis, and Dr. A. Volkov. In addition, the support of the U. S. Department of Energy and the hospitality of the Alexander von Humboldt Foundation, the Institute for Theoretical Physics (Giessen), the Hahn-Meitner Institute (Berlin), the Institute for Kernphysik (Darmstadt), the University of Toronto, the Institut Physique Nucleaire (Orsay), and the Centre d'Etude Physique (Saclay) is gratefully acknowledged.

APPENDIX: CONSERVATION OF ENERGY

In this Appendix we consider several aspects of the conservation of energy for systems described by single-determinantal wave functions. We recapitulate the (average) conservation of energy in the conventional TDHF theory. For TD-$\mathcal{S}$-HF we note that the average energy is constant for each asymptotic channel state of TD-$\mathcal{S}$-HF not only as it propagates in time, but also, by virtue of the time-averaged orthogonality of the different channels, under the statistical interpretation of these states as (potentially) able to transform among themselves. Finally, we consider the very special case of two determinantal eigensolutions of the exact Hamiltonian and show without reference to their spatial orthogonality that their overlap, averaged over a time interval ΔT, is zero unless their energies are approximately (i.e., within $\sim\hbar/\Delta T$) equal.

Thus although no theorem has been found guaranteeing the vanishing of matrix elements $\overline{\mathcal{S}}_{fi}$ between states of different energy, there exists one example where *approximate* energy conservation prevails for an analogous amplitude, in accord with the usual time-energy uncertainty principle, offering promise of future generalization of such an approximate energy conservation to all $\overline{\mathcal{S}}$-matrix elements.

Conservation of energy in the TDHF theory

It is an immediate property of any exact solution $\Psi(t)$ of the time-dependent Schrödinger equation that the expectation value of the energy is constant in time:

$$d\langle\Psi|H|\Psi\rangle/dt=\dot{E}=\langle\dot{\Psi}|H|\Psi\rangle+\langle\Psi|H|\dot{\Psi}\rangle \tag{A1}$$

$$=(i\hbar)^{-1}\langle\Psi|[H,H]|\Psi\rangle\equiv 0\,. \tag{A2}$$

Likewise for any solution $\Phi_i(t)$ of the time-dependent Hartree-Fock equation (3), the time derivative of the energy expectation value is given by

$$d\langle\Phi_i|H|\Phi_i\rangle/dt=\dot{E}=\langle\dot{\Phi}_i|H|\Phi\rangle+\langle\Phi_i|H|\dot{\Phi}_i\rangle \tag{A3}$$

$$=(i\hbar)^{-1}\langle\Phi_i|[H,\mathcal{H}]|\Phi_i\rangle\,, \tag{A4}$$

and as we see below, the right-hand side vanishes identically:

$$=(i\hbar)^{-1}\langle\Phi_i|[H,H]|\Phi_i\rangle\equiv 0\,. \tag{A5}$$

This follows from the one-body structure of the Hartree-Fock Hamiltonian $\mathcal{H}$. It has nonzero matrix elements only between the solution Φ_i and (besides Φ_i itself) its one-particle, one-hole excitations. Moreover, the latter are identical with the corresponding matrix elements of H. That is,

$$\langle\Phi_i|\mathcal{H}|\chi_n^\sigma\rangle=\langle\Phi_i|H|\chi_n^\sigma\rangle\delta_{n1}+E_{\mathrm{HF}}\,\delta_{n0} \tag{A6}$$

defines *all* the matrix elements of $\mathcal{H}$ from Φ_i to the (complete) set of intermediate state determinants, where χ_n^σ is the σth n-particle n-hole state with respect to the determinant $\Phi_i=\chi_0^i$. From (A6) and (A4), the result (A5) follows immediately.

Other constants of the motion in TDHF

Similarly if $\mathcal{O}$ is the one-body operator for any physical observable which is an exact constant of the motion (i.e., commutes with H), its expectation value will also be constant in the TDHF approximation, since its time derivative

$$d\langle\Phi_i|\mathcal{O}|\Phi_i\rangle/dt=\dot{\mathcal{O}}=(i\hbar)^{-1}\langle\Phi_i|[\mathcal{O},\mathcal{H}]|\Phi_i\rangle \tag{A7}$$

reduces, by (A5) and the one-body and Hermitian properties of $\mathcal{O}$, to the identity,

$$\dot{\mathcal{O}}=(i\hbar)^{-1}\langle\Phi_i|[\mathcal{O},H]|\Phi_i\rangle\equiv 0\,. \tag{A8}$$

Energy conservation in TD-$\mathcal{S}$-HF: Asymptotic

In Sec. VII E we analyzed the orthogonality properties of asymptotic reaction channels built on periodic TDHF droplet states and found that for a discrete energy spectrum the channel states would be orthogonal unless Eq. (55) were honored:

$$E_f^{(1)}+E_f^{(2)}+S_f^{(1)}\hbar\omega_f^{(1)}+S_f^{(2)}\hbar\omega_f^{(2)}$$
$$=E_{f'}^{(1)}+E_{f'}^{(2)}+S_{f'}^{(1)}\hbar\omega_{f'}^{(1)}+S_{f'}^{(2)}\hbar\omega_{f'}^{(2)}\,. \tag{A9}$$

Here $E_f^{(1)}$ is the energy of fragment number 1 in its periodic state of channel $\{f\}$, the frequency $\omega_f^{(1)}$ is the fundamental frequency of the periodic state (equal to its period divided by 2π), and $S_f^{(1)}$ is a function which takes on integral values only.

Apart from an accidental degeneracy between one energy and the sum of another energy plus one of its integral overtones, Eq. (A9) is satisfied only if the total energy in channel $\{f\}$ is identical with the total energy in channel $\{f'\}$. But when (A9) is not satisfied, $z_{ff'}$ of (44) cannot vanish and the channel orthogonality property (53) follows. Thus, we see that the time-averaged overlap is zero between asymptotic states of different energy. It follows that energy is conserved during the asymptotic channel propagation of the TD-$\mathcal{S}$-HF states, as interpreted under Axiom II of Sec. V E.

This energy conservation is, of course, a conservation on the time average as the discussion of Sec. VII E leading to Eq. (A9) above clearly indicates and, indeed, as are all the asymptotic implications of the TD-$\mathcal{S}$-HF method for channels involving droplet vibrations with finite period.

Energy conservation during the collision interval

With regard to the propagation of the TD-$\mathcal{S}$-HF states during the collision interval, consider the $\overline{\mathcal{S}}$-matrix defined by Eq. (21):

$$\overline{\mathcal{S}}_{fi}=(\Delta T)^{-1}\int_{-\Delta T/2}^{+\Delta T/2}\langle\Phi_f(t')|\Phi_i(t')\rangle dt'\,, \tag{A10}$$

where we have written $\Delta T=T_2-T_1$, and centered the time interval at $t'=0$.

Unfortunately, no model problem is available for which (A10) could be explicitly analyzed.

Therefore we turn to an amplitude analogous to (A10), but involving bound states, and consider the case where some time-independent determinants Φ_f and Φ_i happen to be eigenstates of the *exact* Hamiltonian,[88] H. That is,

$$H\tilde{\Phi}_g = E_g\tilde{\Phi}_g \quad (g=i,f)\,. \tag{A11}$$

Then the time-dependent solutions are given by

$$\Phi_g = \tilde{\Phi}_g[\exp(-iE_gt/\hbar)] \quad g=i,f, \tag{A12}$$

and $|\mathcal{S}_{fi}|^2$ reduces to the form

$$|\mathcal{S}_{fi}|^2 = |\langle\tilde{\Phi}_f|\tilde{\Phi}_i\rangle|^2\{(2\hbar/\Delta T\Delta E)^2\sin^2(\Delta T\Delta E/2\hbar)\} \tag{A13}$$

where $\Delta E = E_f - E_i$. The second factor in (A13) approaches the value 1 or 0 for $\Delta T \to \infty$, depending on whether $\Delta E = 0$, or not. For finite ΔT it is nearly equal to 1 when $\Delta E \ll \Delta T/2\hbar$ and small when $\Delta E \gg \Delta T/2\hbar$. Thus one concludes that $\mathcal{S}_{fi}$ honors in this case an *approximate energy conservation law* in that it describes transitions from state i to state f of substantial probability only when their energies obey the inequality

$$E_f - E_i \leq (\hbar/2\Delta T)\,. \tag{A14}$$

For the more general case when $\tilde{\Phi}_f$ and $\tilde{\Phi}_i$ are not eigenstates of H the functions will have the form

$$\Phi_g = [\exp(-iE_gt/\hbar)]\tilde{\Phi}_g(t)\,, \tag{A15}$$

where $\tilde{\Phi}_g$ is here also time dependent. Then the spatial overlap factor cannot be extracted from the time integral and the approximate energy conservation relation (A14) is not immediately implied.

Still, the energy phase factor in (A15) and the time dependence of $\tilde{\Phi}_g(t)$ are not closely correlated physically, since the time dependence of $\tilde{\Phi}_g(t)$ reflects the complicated interaction dynamics among the A-interacting nucleons. Therefore, one might seek an energy conservation law of a statistical nature, under which the $\mathcal{S}_{fi}$ overlaps, although not guaranteed always to be zero between states of different energy, might nevertheless reflect the impact of the factor $\exp[i(E_f - E_i)t'/\hbar]$ by exhibiting small values between states of energies whose difference substantially exceeds the limit $\hbar/\Delta T$.

Clearly, a numerical experiment to study the energy conservation in a fully time-dependent example would be most illuminating.

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[12] Except for those two-nucleon interactions for which the exchange contributions to the average potential happen to vanish or are neglected. See Refs. 10 and 11.

[13] Extensive references can be found in Refs. 10 and 11.

[14] James J. Griffin and P. C. Lichtner, in Proceedings of the IV International Conference on Gross Properties of Nuclei, Hirschegg, Kleinwalsertal, Austria, 1976 (Technische Hochschule Darmstadt, West Germany), p. 21; University of Maryland Technical Report No. 76–096 (unpublished).

[15] Preliminary reports of the present work can be found in Refs. 16 and 17 and an outline summary in Ref. 18.

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[27] R. J. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), Chap. 6.

[28] E. P. Wigner, *Group Theory and Its Applications to the Quantum Mechanics of Atomic Spectra*, translated by J. J. Griffin (Academic, New York, 1959), especially Chap. 6.

[29] We include among the "periodic" solutions the stationary solutions, considering them to be periodic with period zero. But note that the periodic droplet states of nonzero period here called periodic for short are not in fact periodic states properly so called, but rather belong to the special class of *quasiperiodic* states which are a product of two periodic functions, a time-dependent space-independent energy phase factor with one period, and a space-dependent factor of a different period [cf. Eq. (36)]. When precision is required we refer to such functions as "phase-quasiperiodic." See especially Sec. IV J. The time-dependent phase factors are fixed, up to an overall "gauge" transformation, by the TDHF variational principle, as discussed in Refs. 30 and 31. See also Ref. 74.

[30] Lichtner *et al.* (Ref. 31) show that the action-integral form of the time-dependent Schrödinger variational principle implies (3) as the *unique* TDHF equation, in contradiction to the long-standing view that the TDHF phase is arbitrary and nonphysical. Reference 31 discusses also the origin of that view in the omission of norm-violating variations from the variational derivation of the TDHF system.

[31] P. C. Lichtner *et al.*, Phys. Rev. C 20, 945 (1979); Phys. Lett. 88B, 221 (1979). An earlier report by these same authors, which preceded their critical study of the variational method, suggested the same phase as a best although not a required, choice (University of Maryland Technical Report No. 78-057, unpublished).

[32] We use the practical physicists' meaning of the term "determines" here, in spite of the fact that the mathematical existence and uniqueness of solutions of the TDHF nonlinear partial differential equations are still subjects for research study (e.g., see Refs. 33–35). Indeed even rigorous statements about the ground state solutions to the *stationary* Hartree-Fock problem for atoms, so long taken for granted in physics, have just recently been rigorously established; cf. Refs. 36–39.

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[55] J. J. Griffin, in *Proceedings of the Second International Atomic Energy Symposium on the Physics and Chemistry of Fission, Vienna, Austria, 1969* (International Atomic Energy Agency, Vienna), p. 3.

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[57] J. J. Griffin and K. K. Kan, in *Proceedings of the Third International Atomic Energy Symposium on the Physics and Chemistry of Fission, Rochester, New York, 1973* (International Atomic Energy Agency, Vienna, 1974), Vol. I, p. 533.

[58] The heavy-ion reaction initializes all the free energy in the one degree of freedom describing the relative motion of the two nuclear centers of mass, an extremely disequilibrized state.

[59] See Refs. 14 and 18 for a discussion of this principle, which states simply that: *A sound theoretical model should yield only information commensurate with its structure*.

[60] C. T. Alonson, *in Proceedings of the International Conference on Drops and Bubbles*, Pasadena, Calif., 1974 (California Institute of Technology, Pasadena, Calif., 1974), p. 139.

[61] J. A. Maruhn, Oak Ridge National Laboratories Report No. CONF-770602, p. 156.

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[63] H. Weidenmuller, in *Proceedings of the Topical Conference on Heavy Ion Collisions, Fall Creek Falls, Tenn., 1977* (National Technical Information Service, Springfield, Va., 1977), Oak Ridge National Laboratories Report No. CONF-770602, p. 199.

[64] Such as Peierls' Theorem (Refs. 65–66) which guarantees that the average (over an ensemble at fixed temperature) free energy is a concave function of every variational parameter so that *every* reduction in the variational integral (i.e., the free energy expectation value) is associated with an improvement in the approximation to the exact solution.

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[67] K.-K. Kan, P. C. Lichtner, and J. J. Griffin, Nucl. Phys. A334, 198 (1980).

[68] It is worth emphasizing that only in the asymptotic region, where the self-consistent potential is well separated spatially into two separate potentials, is it clear that these cross channel correlations are *spurious*. In the interaction region, the cross channel correlations describe within the single-determinantal restriction physically plausible couplings analogous to those among the components of the "resonating group" wave function (Ref. 25), or of the components of a multiparameter generator-coordinate wave function (Ref. 69). On the other hand, even these correlations might sometimes be physically spurious artifacts of the single-determinantal restriction. The spurious correlations of concern in this research are in fact all *post-breakup spurious cross channel correlations*, properly so called.

[69] J. J. Griffin and J. A. Wheeler, Phys. Rev. 108, 311 (1957).

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[72] Note that in conventional initial-value TDHF theory there is no guarantee that the late-time post-reaction wave function splits into separated subdeterminants with integral nucleon number. Indeed, numerical experiments (see Ref. 8) on nuclear reactions indicate the contrary. We note that rigorous global analysis has so far lead only to the result that the initial value TDHF solutions with negative energy do not approach zero as $t\to\infty$ (Ref. 34).

[73] Besides being stationary, the Hartree-Fock ground state is also *stable* in that no small perturbation of it will grow spontaneously. Many other stationary solutions of the Hartree-Fock equations exist, some of which are surely unstable. We here have not invoked stability as a criteria upon asymptotic reaction channel functions. Nevertheless, we believe that the stability properties of the channel functions deserve careful study, and might emerge as a suitable criterion, in addition to those used here, for asymptotic states.

[74] We note that *almost-periodic* solutions, although sharing many mathematical properties with periodic (or quasiperiodic) solutions, also exhibit a qualitative practical distinction: lacking a well-defined period (or periods) of periodic (or quasiperiodic) functions, they cannot be adequately sampled by some finite set of initial conditions selected to characterize the behavior during the period. Nor can the time-averaged values they describe be certified as calculable over some specific finite interval, defined in the periodic (or quasiperiodic) case by the interval including many periods. One is unable to guarantee, therefore, that almost-periodic solutions can in practice meet the initialization requirements (A) for an acceptable reaction channel. Thus there follows directly from the initialization principle a compelling practical distinction between the almost-periodic and the periodic solutions as prospective reaction channel wave functions. Additionally, the expectation that the periodic solutions alone (or perhaps even, as discussed below in Sec. VII N, some discrete subset of them) promise to provide a complete set encourages the presumption that the full set of almost-periodic solutions is superfluous.

[75] If the solutions were not localized the strength of the mean field would be correspondingly diluted, and the solution would be grossly irrelevant to bound states of physical reactants. However, it would be premature to conclude that because the determinants are always spatially localized the description is necessarily a classical one: wave packets, even when localized can adequately describe such interference phenomena as distinguish the quantal wave mechanical Schrödinger theory from the classical mechanics.

[76] In addition to its time-dependent phase relative to other wave functions, as discussed in Ref. 31.

[77] The fact that these are *asymptotic* states allows this limit to honor consistency: R_s must be chosen large enough to guarantee the desired degree of accuracy.

[78] We treat all packet widths w_f as negligible in the pre-

sent discussion, a simplification which must finally be more carefully reviewed. Thus, any implications which depend essentially upon differences in t_f less than or comparable to $w_f/|\vec{v}_f|$, or upon differences in $|\vec{L}_f|$ less than or comparable to $w_f A_1|\vec{v}_f^{(1)}$, must be reinvestigated for the effects of packet width and structure.

[79] Recall that conditions (a) through (d) of Sec. VIIE are assumed here to be already satisfied. They imply that the translation kinetic energy is identical in channels $\{f\}$ and $\{f'\}$. For this reason these energies have already been canceled from the right and left sides of Eqs. (54) and (55).

[80] K. K. Kan has exhibited certain periodic TDHF solutions for a specific model problem. In that case, the gauge invariant periodic solutions have a discrete and not a continuous-energy spectrum suggesting that the continuous-energy vibrational spectrum need not be characteristic of TDHF periodic solutions. On the other hand, Kan's model exhibits strong "accidental degeneracy" in the present terminology so that its orthogonality properties require further study. See also Refs. 89 and 90.

[81] See, for example, Refs. 82–83 regarding experimental studies of classical droplet collisions, their theoretical description (Ref. 84), and their possible analogies with nuclear heavy-ion reactions (Refs. 84–85).

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[83] R. W. Park, Ph.D. thesis, University of Wisconsin, 1970 (University Microfilms Inc., Ann Arbor, Mich., 1979).

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[85] J. B. Natowitz and M. B. Namboodiri, Phys. Rev. C 12, 1678 (1975).

[86] Again, except for possible accidental degeneracies excluded in Chap. VII.

[87] We follow Ref. 30 here and use the word "closed" to denote descriptions where only one TDHF solution occurs in the description.

[88] In Ref. 30, one nontrivial Hamiltonian is exhibited whose eigenstates are determinants. There also the relative time-dependent phases implied by (13) are shown to be uniquely implied by the TDHF variational principle.

[89] See the note added in proof and the more recent developments of Refs. 90 and 91.

[90] K.-K. Kan, P. C. Lichtner, M. Dworzecka, and J. J. Griffin, Nucl. Phys. A332, 109 (1979); also, in *Time Dependent Hartree Fock Method*, edited by P. Bonche *et al.* (Editions de Physique, Orsay, France, 1979), p. 69; Nucl. Phys. (to be published); Phys. Rev. C 21, 1098 (1980).

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