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NUCLEAR MATTER FLOW: FLUID DYNAMICS OF SMALL, FINITE SYSTEMS

James J. Griffin[†*††]
Department of Physics and Astronomy
University of Maryland, College Park, Maryland 20742 U.S.A.

ABSTRACT

Those qualitative properties of nuclei, and of their energetic collisions, which seem of most importance for the flow of nuclear matter in these collisions are listed and briefly discussed. It is suggested that nuclear matter flow is novel among fluid dynamical problems. The name, Nuclear Fermi Dynamics, is proposed as an appropriate unambiguous label. The Principle of Commensurability, which suggests the measurement of the theoretical content of an approach against its expected predictive range is set forth and discussed. Several of the current approaches to the nuclear matter flow problem are listed and subjected to such a test. It is found the the Time-Dependent Hartree-Fock (TDHF) description, alone of all the major theoretical approaches currently in vogue, incorporates each of the major qualitative features within its very concise single mathematical assumption.

Some limitations of the conventional TDHF method are noted, and one particular defect is discussed in detail: the 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. It is noted that the *structure* of TD-$\mathcal{S}$-HF can be applied to a more general class of non-linear wave mechanical problems than simply TDHF.

Physical requirements minimal to assure that TD-$\mathcal{S}$-HF represents a sensible reaction theory are utilized to prescribe the definition of acceptable asymptotic channels. That definition, in turn, defines the *physical range* of the TD-$\mathcal{S}$-HF theory as the description of collisions of certain mathematically well-defined objects of mixed quantal and classical character, the "TDHF droplets."

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*The TD-$\mathcal{S}$-HF reformulation is a collaborative effort with Drs. P. Lichtner and M. Dworzecka. Dr. T. Tamura and Dr. Kit-Keung Kan have also recently studied the physical content of TDHF. We appreciate conversations with them and a prepublication copy of their work.
††Invited Paper presented at the International Symposium on Nuclear Collisions and Their Microscopic Description, Bled, Yugoslavia, September 26 - October 1, 1977. A preliminary report of this work can be found in ref. [36].

INTRODUCTION

This report comprises four subsections, with subtitles as follows:

IA. IB. Nuclear Fermi Dynamics and the Commensurability Critique. For example,

II. One Limitation of Conventional Numerical TDHF: Spurious Cross Channel Correlations, which suggests the

III. Reformulation of the Theory into TD-$\mathfrak{L}$-HF, whence one defines

IV. "Channels" in the TD-$\mathfrak{L}$-HF Theory and its Physical Range: the collisions of the (mixed quantum-classical) "TDHF Droplets."

I.A. NUCLEAR FERMI DYNAMICS

RELEVANT PROPERTIES OF NUCLEI

In part I, we discuss briefly three nuclear properties and two circumstances of nuclear heavy ion collisions which promise to be of qualitative significance in the description of the matter flow during such collisions. Table I lists these items and identifies them briefly. Of the three, the SMALL and FINITE properties are two which are unique to nuclei and promise to set nuclear matter dynamics apart from the flow of matter in other physical systems.

The nucleus is said to be "small" by virtue of the fact that the dimensionless size parameter, R/λ (where λ is the mean free path of a nucleon inside the nucleus) is less than one(*), for a substantial range of low nuclear temperatures(†).

The long mean free path is, of course, the result of the Fermi statistics of nucleons and the resulting Pauli exclusion principle. This same property provides the theoretical validation of the shell model description of nuclear structure [5-6]. We believe, therefore, that it warrants prime consideration in the construction of any theory of nuclear matter flow.[7].

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* This mean free path, λ, can be estimated to be $\sim$13 Fm for neutrons incoming with 10 MeV kinetic energy on the basis of the imaginary part of the optical model *inside the nucleus* as fit to measurements by Greenlees and Bechetti. [1]. Such a value is qualitatively substantiated by the theoretical calculations of Vinh-Mau and Bouyssy [2].

† Kind, et al., [3] have calculated as a function of temperature the mean path of a nucleon in a nuclear degenerate Fermi gas of temperature, T, and report that the mean free path exceeds the nuclear radius for temperature up to about 7MeV, for incoming nucleon energies up to 35 MeV. Collins, [4] is currently re-analyzing this problem. In terms the theory of Fermi Liquids, Wegman [4a] has especially emphasized the importance of the long mean free path for nuclei.

The SMALLNESS of nuclei, on the other hand, offers a substantial obstacle to any assumption of local equilibrium in any small volume inside the nucleus, and would seem to exclude the possibility of a

(Text continues on following page).

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TABLE I: SALIENT FEATURES OF NUCLEAR FERMI DYNAMICS

A. Three Nuclear Properties

1. FERMI → SMALL, $R/\lambda < 1$; implies

   No Local Equilibrium
   Collisions of Particles with Walls are Crucial

2. FINITE-A, GRANULAR; implies

   STRUTINSKY GENERALIZED SHELL EFFECTS on
   POTENTIAL, INERTIAL, and DISSIPATIVE parameters

3. LIQUID-SELF-BOUND:

   System responds self-consistently to its own motion.

B. Two Circumstances

1. NON-EQUILIBRIUM ↔ DISSIPATIVE

   Suppressed degrees of freedom serve as dissipative sink

2. MASS-DYNAMICAL ↔ GLOBAL

   Matter flow substantially alters average field during process.

hydrodynamical description(*) via equations of the Navier-Stokes type. For such theories deal with intensive variables which are assumed to vary smoothly across the nucleus.

In addition, NUCLEAR SMALLNESS focuses one's attention on the collisions of nucleons with the walls of the nucleus, since these are the *only* collisions left when the mean free path becomes very large. This qualitative feature [7] is elevated to an exclusive role in the "wall formula" recently recommended by W. J. Swiatecki [10], and plays an important part in the various other one body approaches to dissipation [11-13].

The second property listed is the FINITE-A, or GRANULARITY property of nuclei which arises from the discreteness of their quantum description. This property leads to spherical [14] and generalized [15] shell deviations of the nuclear collective potential energy from its smooth liquid drop value. It arises from the fact that A ($\sim 10^2$) particles allow substantial relative fluctuations from a smooth average as compared with a true many-body system ($A \to \infty$). For macroscopic systems with $A \sim 10^{23}$, e.g., the generalized shell corrections would be much smaller, relatively, and the smooth liquid drop limit much more nearly realized.

We already know that in nuclear physics these generalized shell corrections are sufficient to effect qualitative alterations on the process of nuclear deformation in reaction processes. Especially in the case of fission they supply the currently accepted basis for understanding the mass asymmetry of the fission of heavy nuclei at low and moderate excitation energy [16-19].

(*) We reserve the word *Hydrodynamical* for *water*-like matter flows, well described by the Navier-Stokes equation. The label, *Fluid Dynamical*, on the other hand, denotes the broadest class of matter flow problem, unrestricted to any particular dynamical equation. It should also be noted that the conservation laws (of matter, energy and momentum) must prevail for any physical system [8], and impose upon any dynamical theory a certain general structure sometimes referred to (we think, imprecisely) as "hydrodynamics." The usage here would replace "hydro" by "fluid," except when the tensors involved in the expressions of the conservation laws exhibit the properties (especially locality) which are assumed in the Chapman-Enskog [9] derivation of the Navier-Stokes equations.

In adition, it has been shown that the inertial tensor for nuclear mass flow will also exhibit Strutinsky-type structure in N, Z, and deformation[20] which can be understood as effecting a locally compressible flow for the nuclear matter[21]. Finally, one must anticipate that in a theory which calculates dissipative parameters from microscopic properties, such parameters also will reflect the effects of Strutinsky's generalized shells(*). Thus, the fact that the nucleus is a GRANULAR system will influence the potential, inertial and the dissipative parameters - which is to say, every aspect - of the ultimate description of nuclear Fermi dynamics.

The third property listed, that the nucleus is a self-bound liquid, emphasizes the fact that as nuclear matter flows the average binding field alters in accordance with the matter distribution. The nuclear flow shares this particular property with other physical liquids, but not with gases, nor with the flow of electrons in an atom, where a strong external field (the Coulomb field of the nuclear charge) is unresponsive to the flow of the electron matter.

RELEVANT CIRCUMSTANCES OF NUCLEAR HEAVY ION COLLSIONS

In addition to the above three nuclear properties, two circumstances of the nuclear heavy ion reactions seem essential. The first is that the colliding system is initially extremely DIS-EQUILIBRIZED - containing, in fact, all of its free energy in the single degree of freedom describing the distance between the two nuclei about to collide. One can therefore be certain that, immediately upon collision, this energy will begin flowing into other degrees of freedom, with a strong tendency towards equilibration. The theoretical description of the subsequent motion, since practical considerations require it to involve some number of dynamical variables less than the complete set, will involve from time to time the transfer of energy, momentum, or other physical quantities into degrees of freedom which are being suppressed in the theory. Such transfers which leave the limited space of the retained variables must be considered "dissipation." We therefore expect to deal ultimately in this problem not simply with one "dissipation" but, rather, with several alternative possible dissipative schemes,

(*) Recent work by Koonin and Randrup [13] discussed in conference [36] relates the dissipation kernel to the trajectories of classical particles. These in turn are connected with the degeneracies of a wave mechanical system by Bloch, Balian et al. [22]. Thus already one specific path for describing the influence of generalized shells upon dissipation parameters is available.

corresponding to the various numbers of explicit degrees of freedom which we may wish to retain in a particular description, the remainder of which, having been suppressed, provide the sinks for the dissipated quantities.

The second important circumstance of hard(*) nuclear heavy ion collisions arises from the fact that the substantial mass flow can occur in such reaction processes on a short time scale, and can, therefore, imply substantial readjustment of the average shell-model field during the time of the collision. This requirement of a knowledge of the nuclear shell model properties over a finite region of nuclear shapes (including shapes describing ruptured configurations) we refer to as the GLOBAL property of such collisions. We contrast it with the fact that traditional nuclear structure studies generally require no more than a knowledge of nuclear properties (and one or two derivatives) at an equilibrium point. This GLOBAL-MASS-DYNAMICAL property may, as the description of nuclear heavy ion collisions moves forward, come to place demands upon our mathematical capacity, which can not be met with the techniques currently available. But it is also possible that the dissipative processes in nuclear Fermi dynamics will be so dominant over the mass flow properties as to substantially alleviate, and even qualitatively alter, the Fermi dynamical problem into a dissipation-dominated process, rather than a kinetic-dominated mass flow problem. This expectation has been vigorously advanced by W. J. Swiatecki, in particular [23].

COMPARISON AMONG SOME CURRENT THEORIES

In Table II, we tabulate four current theoretical approaches to nuclear heavy ion collisions, Time-Dependent Hartree-Fock[24], Navier-Stokes Hydrodynamics [25], Transport Theory [26] (including [10] the "window formula") and the "wall formula" [10], and the five features just discussed. A "Yes" is entered for each feature which a given theory meets; a "No" for each feature which a given theoretical approach omits. In a few cases neither a Yes nor a No seems adequate:

(*) The emphasis throughout this talk is upon the matter flow, and therefore the "soft" long-distance collisions of heavy ions are not the focus of attention.

TABLE II: QUALITATIVE PROPERTIES INCORPORATED INTO VARIOUS THEORIES

Property: \ Theory:	*TIME DEPENDENT HARTREE-FOCK*	*NAVIER-STOKES HYDRODYNAMICS*	*TRANSPORT THEORY (including Window Formula)*	*WALL FORMULA*
SMALL-FERMI ($\lambda > R$)	Yes	No	—(a)	Yes?(b)
FINITE A (Genalized Shells)	Yes	No	No	No
LIQUID (Self-bound)	Yes	Yes	No	No
GLOBAL MASS-DYNAMICAL	Yes	Yes	No	—(c)
NON-EQUILIBRIUM DISSIPATIVE	Yes	Yes	Yes	Yes

a)b)c) refer to notes so labelled in the discussion in the text.

(a) The transport theory description of energy charge and mass equilibrization between two fragments in deep inelastic contact might describe systems with long mean free paths or short mean free paths by incorporating their respective effects into its phenomenological transport coefficients;

(b) The wall formula [10](which is an extension of the piston model [11] to the complete 4π nuclear solid angle) incorporates the long mean free paths by omitting all collisions *except* those with the wall. On the other hand, it is a classical description and incorporates no further effects of the Pauli exclusion effects upon the Fermi particles. Therefore the response: "Yes?."

(c) The wall formula is narrowly aimed at dissipation. Therefore it does not imply, nor exclude, any particular matter flow description.

We emphasize that the successful incorporation of all the important qualitative physical aspects into a single concise assumption, which the Time-Dependent Hartree-Fock method achieves, is no assurance that the resulting description will adequately describe observed nuclear data. Indeed, Commensurability, as discussed below, might dim one's hope to get so much from so little. Even so, the TDHF is of great interest, precisely because of the very economy of its assumptions, as a theorists' theory, to teach one how to look at problems in Fermi dynamics and what reasonably to expect from them. It is for this reason, rather than from an expectation of any successful confrontation between TDHF and observed data, that we devote some considerable discussion to this model below.

I.B. COMMENSURABILITY IN THE ASSESSMENT OF DESCRIPTIONS OF COMPLICATED PHENOMENA

We note that one can formulate the present outlook consciously into a method of assessment of theories for complicated processes such as the present physical problem poses. This method employs The Principle of Commensurability[27],stated as follows:

A sound theoretical model should only yield information commensurate with its input and its structure.

We consider this statement to be self-evident. However, it implies immediately the practical corollary that models which give too much may be erroneous, or may involve hidden assumptions. In addition it leads one to evaluate theoretical models, and especially complicated

models, by emphasizing the "commensurability" between the input, the structure and the predictive capacity of the model. Such an evaluation can be helpful in focussing the search for limitations and/or shortcomings in any proposed theoretical description.

Finally, for a model characterized completely by *mathematical* assumptions, the principle of commensurability suggests the question: What is the *physical* range of the model? This question becomes the more difficult (and its answer the more useful), the more concise and compact is the assumptive mathematical basis of a given model. In particular, as Table I illustrates forcefully, the single-determinant assumption of the Time-Dependent Hartree-Fock description provides an appropriate specific example of a very concise assumptive axiomatic basis for a model, which is able (cf. Table II) to incorporate an impressive range of appropriate physical property, but whose *physical* implications are not immediately transparent.

II. LIMITS OF THE TDHF DESCRIPTION OF COMPLEX REACTIONS: SPURIOUS CROSS CHANNEL CORRELATIONS

CONVENTIONAL TDHF DESCRIPTION

We turn now to a discussion of the numerical Time-Dependent Hartree-Fock method [24] which so economically and completely incorporates the qualitative features of Nuclear Fermi dynamics into the single assumption that the exact solution will be approximated as

$$\Psi \sim \Phi \text{ , a single determinant .} \tag{1}$$

This assumption, imposed as a restriction on the variational principle whose unrestricted variation yields the Time-Dependent Schrödinger Equation,

$$i\hbar\dot{\Psi} = H\Psi \tag{2}$$

leads to the *Time-Dependent Hartree-Fock Equation*, [28]

$$i\hbar\dot{\Phi}(t) = \mathcal{H}^{HF}(\Phi(t)) \cdot \Phi(t) \tag{3}$$

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

$$\Phi(t)\Big|_{t=t_i} = \Phi_o \tag{4}$$

gives the initial condition, whence equation (3) specifies the solution $\Phi(t)$ for all subsequent times.

Thus the TDHF problem, once posed and once subjected to initial conditions, *appears to be* an axiomatically complete structure whose predictions are inexhorable and unalterable. Indeed it is this very compact and closed character of the TDHF problem which enhances its interest for theoretical analysis. For, once the initial values are given and the method of propagation forward in time is prescribed, one seems committed to a specific outcome and is allowed, apparently, no freedom for reinterpretation or creative restructuring of the physical content of the description. One could easily be persuaded that substantial phenomenological success in such a tightly constrained theoretical realm should be considered as very significant. (By Commensurability, on the other hand, one expects that such a drastic simplification of the Schrödinger theory could not fail to lose some essential features of the nuclear physics.)

In spite of its apparent rigidity, we shall here propose a reformulation of the TDHF description for problems involving reaction from and into asymptotic reaction channels. For, as a reaction theory, the TDHF is not so inflexible as it might at first seem. In fact, its basic assumption that the wave function shall be a single determinant can be imposed on reactions in more than one way. We propose here a reformulated method which is physically more reasonable than the more direct method used so far in numerical analyses by the TDHF method.

We should mention also the practical basis for great current interest in Numerical TDHF: the fact that the numerical solution of the TDHF problem with nuclear model forces of the Skyrme type [29,30] was shown in recent years to be possible and became therefore the object of substantial effort, and that it continues to command considerable attention [24]. Thus, TDHF is now a practical object for numerical experiment.

We emphasize that in spite of the remarkable incorporation of the main qualitative nuclear properties into the TDHF method (as exhibited in Table II), the method is still an *approximate* method. Its restriction to a single determinant limits the accuracy of TDHF in each of the three phases of its time dependent description [27]:

(i) The specification of the initial wave function $\Psi_1(t_1)$ by a single determinant approximation is 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);

*Items (i) and (ii) are discussed further in references [31-32].

(iii) the post-breakup determinant, $\Phi(t)$ $(t >> 0)$, is too simple to describe the many channels of the exact outgoing state, and, to date, lacks any specific proposed interpretation.

SPURIOUS CROSS CHANNEL CORRELATIONS

Here we focus upon the third item, and a remedy for the 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 [33]a "coherent superposition of outgoing channels." The available reaction channels correspond to different pairs of nuclei, and/or for each pair a range of possible excited states, 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 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 that single determinant, results for a multi-channel 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." These spurious interactions exert a distorting influence on the physical content of the final phase of the reaction - a phase which ought to be very simple since it involves merely the translation in space of well-separated fragments which have been formed from the reaction process.

Consider $\Phi(t)$ 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:

$$\Phi(t) = \sum_f w_f \Psi_f(t) \text{ for } t >> 0 . \qquad (5)$$

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

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

$$= |w_{O-O}|^2\ V_{HF}^{O-O} + |w_{Si-He}|^2 [V_{HF}^{Si-He} + V_{HF}^{He-Si}] \tag{7}$$

Here V_{HF}^{O-O} denotes the self-consistent potential for a 32 x 32 determinant built by anti-symmetrizing two 16 x 16 subdeterminants each describing ^{16}O in its Hartree-Fock ground state well separated in space. This is exactly the potential which arose in the incoming channel of this same reaction. On the other hand, V_{HF}^{Si-He} is the self-consistent potential for a 32 x 32 determinant built from a 4 x 4 determinant describing the ^4He ground state and a 28 x 28 determinant for ^{28}Si. Equation (7) demonstrates the fact that *the Hartree-Fock potential even in the asymptotic region, is a mixture of potentials for the several channels it attempts to describe.*

A very similar argument shows that only channels which *happen to have* the same 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.

We conclude from the existence of these spurious cross channel correlations in the late stages of a multi-channel process as described by TDHF, that *the TDHF description, as conventionally applied, is not able to provide a self-consistent propagation in time for any one of several outgoing open channels in the final stages of a reaction process.* Only in the (exceptional) case of a single outgoing channel can the conventional TDHF state provide the best single determinant description of any particular pair of separating fragments.

From these considerations we are led to propose the following 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.

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

We first make a simple renotation of the Time-Dependent Hartree-Fock wave function evolved from the initial state, i, by the Hartree-Fock propagation forward in time. Let

$$\Phi(t) = \Phi_i^{(+)}(t) = U_i^{(+)}(t,t_i)\ \Phi_i^{(0)}(t_i) \tag{8}$$

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

$$\phi_f^{(-)}(t) = U_f^{(-)}(t,t_f)\phi_f^{(0)}(t_f) \tag{9}$$

to be the wave function evolved backwards in time via a similar, but time-reversed TDHF process from $\phi_f^{(0)}(t_f)$.

THE (TIME-DEPENDENT) CURLY-$\mathcal{S}$ MATRIX

We then construct the following analog of the scattering matrix:

$$\mathcal{S}_{fi}(t) = \langle\phi_f^{(-)}(t)|\phi_i^{(+)}(t)\rangle \ . \tag{10}$$

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 (time-independent) S-matrix element which gives the amplitude for the wave packet evolved from the initial state, i, to be found in the state which will evolve to the final state, f. We therefore consider $\mathcal{S}_{fi}(t)$ to be the amplitude that the TDHF "state," $\phi_i^{(+)}(t)$, is found at time t to be the TDHF "state," $\phi_f^{(-)}(t)$, which will *evolve under TDHF to the final state* $\phi_f^{(0)}$ *at* $t = t_f$, *without spurious cross channel correlations with channels other than f*. Then we propose that

$$\bar{\mathcal{S}}_{fi} = \frac{1}{2T}\int_{-T}^{+T} dt\, \mathcal{S}_{fi}(t) \tag{11}$$

(where (-T,T) is the interaction interval, during which neither Φ_i nor Φ_f is "spuriously" describing multi-channel processes)

(*) The time derivative of $\mathcal{S}$ in equation (6) can be estimated from those of Φ_i, Φ_f to be of order $(i\hbar)^{-1}$ times of the difference between the corresponding matrix elements of the two distinct Hartree-Fock Hamiltonians, H_i and H_f, at time, t. Since their diagonal elements are ~ -8 A$\approx 10^3$MeV, this derivative might easily have a magnitude as large as (100 MeV)/$\hbar \approx 10^{23}$/sec. We therefore consider any attempt to utilize $\mathcal{S}(t)$, unaveraged in time, as futile.

describes the (relative) amplitude that the TDHF state i which evolves from $\phi_i^{(0)}$ at $t = t_i << 0$ will be found in the state, $\phi_f^{(0)}$, at $t = t_f >> 0$.

Normalized (since there is no structural compulsion for unitarity in this theory) for the incoming channel i, this becomes

$$\hat{\mathcal{S}}_{fi} = \mathcal{S}_{fi} / [\sum_f \mathcal{S}^*_{fi} \mathcal{S}_{fi}]^{1/2} , \qquad (12)$$

the operational analog of the unitary S matrix in the TD-$\mathcal{S}$-HF theory. Equation (12) completes the required reformulation of the time-dependent reaction theory within the Hartree-Fock framework.

Note that the result (11) applies independent of the particular prescription for the time evolution operations, $U^{(\pm)}$, in equations (8) and (9). It represents therefore an alternative to the use of equation (8) 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, equation (10), is expected to apply.

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

1. The once only multi-outgoing-channel TDHF calculation of $\phi_i^{(+)}(t)$ is replaced by one time-reversed incoming calculation of $\phi_f^{(-)}(t)$ *for each final channel.*

2. A time integral of the overlap

$$\langle \phi_f^{(-)} | \phi_i^{(+)} \rangle = \mathcal{S}_{fi}(t) \qquad (13)$$

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

3. *No spurious cross channel correlations* enter into $\mathcal{S}_{fi}$: separated configurations are propagated only by single-channel self-consistent Hartree-Fock Hamiltonians.

It is remarkable that this reformulation of the TDHF description for multi-channel processes is able still to conform to the requirement that each wave function at each moment be described as a single determinant. Still, it obviates the spurious correlation difficulty of a single determinantal description of a multi-channel physical situation - a difficulty which seems inescapable in the straightforward time-integration of the TDHF equation from the initial incoming state to a

postbreakup time. Since here a time-reversed calculation is used to propagate each of the outgoing configurations backwards into the interaction region, 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 fits naturally with the time reversal invariance of the 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 direct TDHF method, in which only the nearly unique initial state needs to be constructed, allows one to evade the question of what labels are required to characterize its asymptotic states.

We turn next to a consideration of what these labels should comprise, and obtain therefrom a statement of what a "channel" in the TD-$\mathcal{L}$-HF description is to specify. The sought after result is a clear and concise definition of the *physical range* of the TD-$\mathcal{L}$-HF.

IV. "CHANNELS" IN THE TD-$\mathcal{L}$-HF REFORMULATION

MINIMAL REQUIREMENTS OF A REACTION THEORY

To have a reasonable reaction theory, we need at least to be sure that our predictions are (a) specific and unambiguous, and (b) that they do not depend upon the distance of the measurement apparatus from the collision region. In Schrödinger theory, these conditions follow at once from the superposition principle, which in turn is guaranteed by the linearity of the theory. For non-linear theories like TD-$\mathcal{L}$-HF or TDHF, however, even such basic properties are not automatic, and cannot be guaranteed unless they have been specifically built into the theory.

Within the TD-$\mathcal{L}$-HF framework, we can attempt to guarantee these requirements by the choice of "reaction channels." Alternatively, one could say that these conditions require a certain specific choice for these channels. Then its rational structure determines the theory's *physical range*, as discussed above. We follow such an approach here.

Specifically, we demand that an asymptotic channel, (f), specify

(i) completely, two well-separated sub-determinants at some (arbitrary) large standard initiation distance R_0, and at the time t_f for the initiation of the channel reaction; and that

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

APPLICATION TO HARTREE-FOCK

We note that condition (ii) can be satisfied only by the Hartree-Fock ground state, or by another state which is stationary with respect to variation of the Hartree-Fock determinantal wave function. Unfortunately, the set of states composed of all such stationary states for a given exact Hamiltonian are not orthogonal. (Their inclusion would imply, according to equation (10), spontaneous transitions to other channels, even in the far asymptotic region.) They would therefore seem to be unsuitable labels for the identification of a set of excitations for the initial (or final) nuclear projectile and target.

Thus the literal imposition of condition (ii), together with the proposed interpretation of $\mathcal{H}^{\rho}_{fi}(t)$ in equation (10), would require that we restrict the range of Hartree-Fock theory to mass and energy elastic scattering of the Hartree-Fock ground state, to the set of (orthogonal) Hartree-Fock ground states corresponding to all the different mass division of a given A-nucleon system, or to some other arbitrarily selected subset of orthogonal stationary states. Such a restriction would trivialize the theory unacceptally(*).

However, the requirement of stability for the asymptotic channel amplitudes against spontaneous change during free translation can be met, perhaps adequately, by requiring that it prevail not instant by instant, but instead only on a time averaged basis.

(*) Note that a Gram-Schmidt orthonormalization of the Hartree-Fock stationary states is self-defeating here, because linear combination of stationary states are not stationary in general, as a result, again, of the non-linearity of the Hartree-Fock problem.

Therefore, we here adopt this alternative: That the condition (ii), requiring no change of the internal wave function as it translates freely in space, be applied not as an exact condition, at every time, but instead only on a time-averaged basis. Then

(iii) *Cyclic, self-consistent oscillations* of the subdeterminants for target and projectile become acceptable in the asymptotic reaction channels, since such oscillations imply no change in the *time-averaged* intrinsic structure as the system translates.

We then arrive at the following set of labels for describing the channel wave function(*) $\phi_f^{(0)}(t_f)$ as follows:

$$(f) \equiv (A_1, S_1, A_2, S_2, \vec{R}_f, \vec{v}_f, t_f; \varepsilon_{\lambda_1}, \phi_{\lambda_1}, \varepsilon_{\lambda_2}, \varepsilon_{\lambda_2}) \ . \qquad (15)$$

This set of labels describes:

1. A single $(A_1+A_2) \times (A_1+A_2)$ determinant constructed by anti-symmetrizing:

2. An $(A_1 \times A_1)$ determinant describing the $S_1{}^{th}$ stationary solution(†) of the isolated A_1-particle Hartree-Fock system., and

3. An analogous $(A_2 \times A_2)$ determinant centered at time $t = t_f$ at some fixed (large!) standard distance, $\vec{R}_f$, in the center of mass frame from the center of mass of A_1.

4. Each subdeterminant at the time t_f describes

   (a) a Hartree-Fock stationary(†) state, labelled S_i, which is

   (b) translating at velocity, $\vec{v}_f$, (relative to its partner in the center-of-mass frame), and

   (c) vibrating (in small TDHF self-consistent oscillations) at its various R.P.A. normal frequencies, ω_λ, with amplitudes ε_λ, and

   (d) at time $t = t_f$ has phase angles, ϕ_λ, for these oscillations.

(*) We restrict ourselves to small amplitudes in the TDHF vibrations, where their properties have been extensively studies. See especially reference [35].

(†) Further consideration leads us to expect cyclic vibrations only about the ground state, because of the instability of other Hartree-Fock stationary states against one or more vibrational degrees of freedom. Thus only the Hartree-Fock ground states occur among the labels S_1, S_2 in equation (15):

We thus arrive at the conclusion that THE PHYSICAL RANGE of TD-$\mathcal{S}$-HF is the collisions of "TDHF Droplets", where a *"TDHF Droplet" is completely defined dynamically by its Hartree-Fock ground state and the classical self-consistent TDHF oscillations*(*) *thereof.*

We note that this statement of the physical content of the TD-$\mathcal{S}$-HF scattering theory indicates that that theory is a description of droplets which exhibit each integral-A ground state, in addition to a set of classical oscillations. We say "classical," since the small amplitude TDHF self-consistent oscillations around a stationary state are allowed to have arbitrary amplitude and phase, since the Time-Dependent Hartree-Fock Theory compels no discretization for these vibrational amplitudes. Of course, one might wish in some cases to quantize these classical vibrations to obtain (in the multi-boson, harmonic oscillator approximation) eigenenergies spaced at intervals, $\hbar\omega_\lambda$ where ω_λ is the frequency of a given R.P.A. mode. Such a decision would represent an addition (indeed, perhaps, a most reasonable one) to the theory, not required by its intrinsic structure.

Thus, we conclude the TDHF mathematics describes the approach, the interaction (including possible mass exchange), and the separation of TDHF droplets, whose stable points are prescribed by the ground state solutions of the Hartree-Fock equations, and whose normal mode frequencies for small amplitude oscillation are prescribed by the R.P.A. frequency spectra of oscillations around the stationary states.

In other words, the TDHF description of nuclear scattering processes replaces the nuclei by a very special kind of fluid droplet, which exhibits both stationary states of discrete energy and self-consistent vibrations around them of continuous energy.

(*) See footnote on preceding page.

Each pair of droplets is specified by the list of numbers, (15), which suffice to characterize uniquely the single determinantal "channel" wave functions at large separation distances (i.e., the dynamical behavior of the determinants as isolated systems) and appropriate translational properties. We thus arrive at the remarkable result that the TD-$\mathcal{L}$-HF reaction theory describes the collision such mixed classical-quantum mechanical TDHF droplets in terms of a *wave mechanical amplitude*, $\mathcal{L}$, calculated from the overlap of two determinantal wave functions. This remarkable result seems sufficiently intriguing to warrant further attention.

V. SUMMARY

To recapitulate the content of this paper we recall that in order to remove the *spurious cross channel correlations*, we were led to reformulate the TDHF reaction theory into the TD-$\mathcal{L}$-Matrix-HF Theory.

The resulting structure overflows the limits of its origins and emerges as a general scheme, equation (11), for extracting reaction amplitudes from (non-linear) time dependent theories for which the superposition principle does not apply, but where the wave function at each instant can still be assumed to define the amplitudes for the results of measurements defined by a complete linearly independent set of wave functions, according to equation (10).

Then certain minimal requirements for the reaction theory to make physical sense prescribes certain properties for the asymptotic channels, which in the small amplitude limit for TDHF vibrations(*), can be satisfied by channels which can be defined by the set of labels (15).

The resulting definition of reaction channels in the new TD-$\mathcal{L}$-HF theory defines its physical range to be the collision of "TDHF droplets", those objects whose structure when isolated is described by the TDHF theory. One thus arrives at the very commensurable conclusion that precisely the physical content of the self-consistent TDHF description of an isolated nucleus can be incorporated into the TD-$\mathcal{L}$-HF theory of reactions - no more, and no less. This clear qualitative characterization of the physical implications of the single determinantal assumption for reaction theories should be useful in measuring the achievements of and in prescribing the expectations for the TD-$\mathcal{L}$-HF reaction theory.

(*) New knowledge of the large amplitude cyclic TDHF vibrations of an isolated TDHF droplets could require alteration of this channel definition without undermining the essential proposal for TD-$\mathcal{L}$-HF; namely, that equation (11) defines the (relative) transition amplitudes for reaction.

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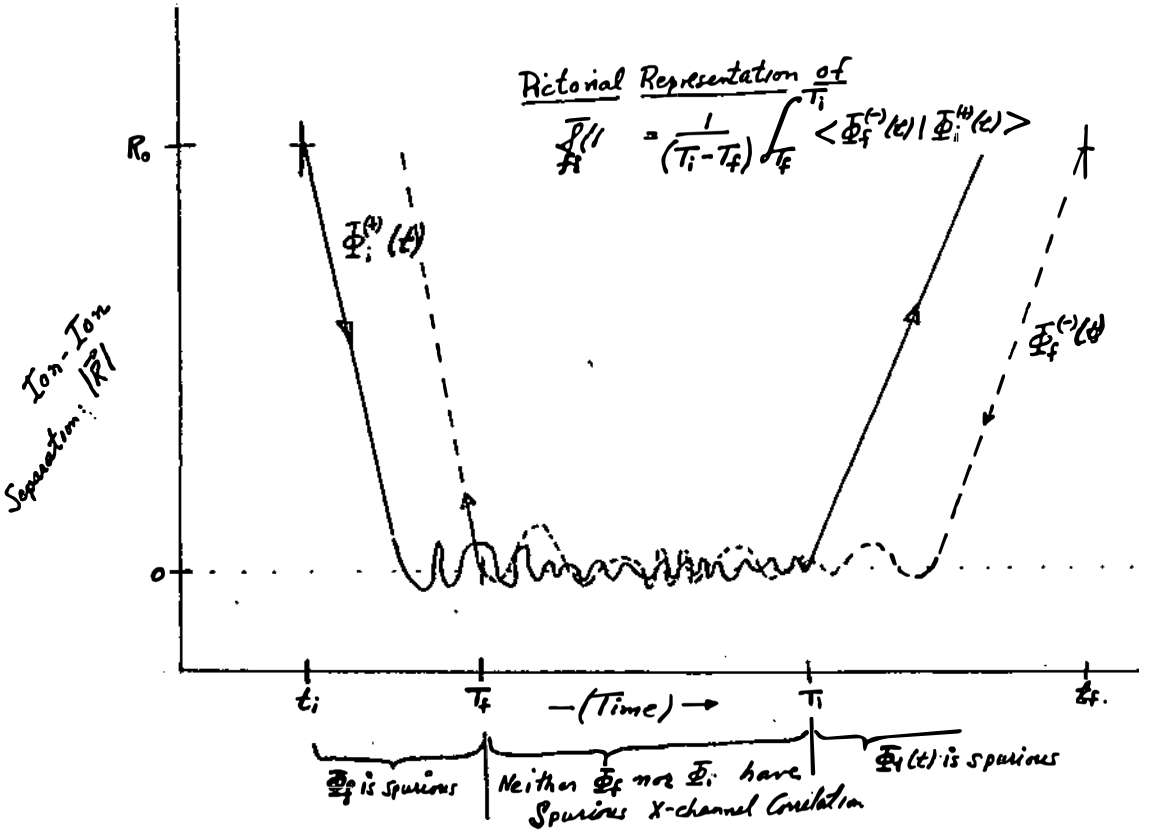

Fig. 1. The interaction interval (T_f, T_i) includes every time when nether $\bar{\Phi}_f^{(-)}$ nor $\bar{\Phi}_i^{(+)}$ exibits spurious cross channel correlations. The lines represent self consistent Hartree Fock evolution forward (solid line) and backward (dashed line). In principal, $|R_o|$, $-t_i$ and t_f are arbitrarily large.

DISCUSSION

B.L. Moiseiwitsch: Could you use a variational principle to obtain an expression for your scattering matrix? This might provide a sounder basis for the theory.

J.J.Griffin: Our construction of the theory has been a heuristic one so far and our effort has been to look for prohibiting reasons against various ones of the choices one might consider making. I do not presently know how to obtain $\mathcal{F}$ or $\mathcal{F}^{\star}$ from any variational principle. I would consider a successful effort to do so as a substantial addition to the theory.

R.J. Philpott: In your expression for the $\mathcal{F}^{\star}$ matrix element, the lapse between the time when the incident channel reaches the interaction region and the time when the exit channel (propagating backwards) reaches the interaction region is not uniquely specified. Nor are the phases of the propagating oscillatory solutions (if any) uniquely specified at these contact points. Since these quantities are likely to affect the value of the matrix element, by what principle should they be chosen?

J.J.Griffin: I should emphasise that the time t_f (or t_i) at which the final (or initial) channel fragment are found at the standard separation distance, $/R_o/$, is a label for the channel, because the fact that the self consistent time-dependent Hartree-Fock solutions are localized in space and time, in contrast to the infinite plane waves usually considered in the Schrödinger stationary state scattering theory. Also the amplitude and the phase of every self-consistent normal mode oscillation of the separated T.D.H.F. droplets must be included in the channel label. Only when all of these quantities have been specified is the information available adequate to specify completely the final (or initial) boundary condition for $\phi_f^{(-)}$ (or $\phi_i^{(+)}$). Cf. Equation (15) of text. The need for these quantities underlines the classical cha-

racter of the T.D.H.F. droplet translation and excitation in the asymptotic region.

Note also that the theory is invariant under an overall translation in time, since only the difference, $(t_f - t_i)$, actually affects the physical results of the theory. One can thus fix t_i once and for all, and let t_f vary over all possible values in order to extract a complete set of physical predictions from the theory.

K. Dietrich: If you let $T \to \infty$ in your expression for the S-matrix it seems to me that you would obtain zero except for very specific channels. The reason is that the relative motion of the fragments (or fragment ensembles) is different in $\phi_f^{(-)}(t)$ and $\phi_i^{(+)}(t)$ for $t \to \pm\infty$. So the result you obtain depends very much on the choice of T which I feel a bit uneasy about.

J.J.Griffin: I agree with your remark entirely. It follows, as you say, that the results depend very much on the choice of the interval (-T,T) of the time integral. But still your question requires the following two classifying remarks. (See Fig. 1. for reference).

a) The choice of the interval (-T,T), - (more precise labelled (T_f, T_i) as in Fig.2.) is fixed in our approach by the requirement that no spurious cross-channel correlations are allowed to enter into the physical results. But for $t > T_i$, $\phi_i^{(+)}$ includes such spurious correlations; and for $t < T_f$, $\phi_f^{(-)}$ includes them. Thus the interval is not freely adjustable.

b) Even if the quantity $\bar{\mathcal{F}}_{fi}$ were in some case to approach zero, the corresponding re-normalized quantity $\hat{\mathcal{F}}_{fi}$ in equation (12) might be finite. In other words, the fact that the physical content of this theory is contained in relative amplitudes among different final channels, or in the ratios, $\bar{\mathcal{F}}_{fi} / \bar{\mathcal{F}}_{f,i}$, requires special cre in interpreting $\bar{\mathcal{F}}_{fi}$ when it becomes very small.

B.G.Giraud: I do not see clearly what is the hierarchy of times implied by this theory. If I understood properly there are probably at least three kinds of times: the periods τ you allow in the channels, the periods τ' of the spurious correlation fluctuations, and the averaging time T. Might it happen that one needs a condition like, say, $\tau' \ll \tau \ll T$, or maybe $\tau' \ll T \ll \tau$?
What happens to delayed transitions, resonances and other isomer states?

J.J. Griffin: Our philosophy has been consistently to keep the self consistency condition and to try to optimize the physical content which it allows the theory to have. In this way we arive at two sets of natural times: (a) The collision intervals (-T, T) defined by the limits of the integral in $\hat{\mathcal{J}}_{fi}$, (b) the periods, $\tau_\lambda = 2\pi/\omega_\lambda$, of the normal mode vibrations of the isolated TDHF droplets.

The collision intervals are chosen to be as large as possible, but not including any region where ϕ_i or ϕ_f is forced to describe more than one reaction channel. They therefore depend upon the channels (i,f). (We note that t_i and t_f the times at which the subdeterminants are separated by the standard (large) distance R_o, are channel labels. By adjusting their difference, e.g. by varying t_f, one can make the interaction interval $2T = 2T_{if}$ to be as small as one chooses, for a given fixed choice of all other channel labels.) They therefore follow from the theory itself, and no condition is evident which needs to be imposed upon them. Note however, that the maximum value of $2T_{if}$ always exceeds the sum of the interaction lifetimes of i and f. Thus "isomers" and "resonances" enter by their elongation of the interaction interval. Also if either the i or f channels, or both, takes an infinite time to break up, then a corresponding interval $2T_{if}$ would become infinite. Thus very long-lived interacting states correspond to "fusion", signalled by an infinite value of the interaction interval, $2T_{if}$.
The periods of the self-consistent oscillations of the isolated T.D.H.F. droplets also follow from the theory itself.

They comprise, (omitting the possibility of decay of the fragments) a discrete infinity of periods, which however seems to have no restrictive effect upon the theory, except for the requirement of a time averaging of the observation of the asymptotic behaviour sufficiently broad in time to allow the accurate Fourier analysis of the asymptotic state.

The third time you mention, τ', associated with the "spurious correlation fluctuations", is, we hope, completely eliminated from the theory by the specific elimination of all wave functions involving spurious cross-channel correlation (i.e. all wave-functions attempting to describe multiple channels in the non-interacting region) from the physically significant quantities of the theory.