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NUCLEAR FERMIDYNAMICS AND T.D.-$\mathcal{S}$-H.F.

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ABSTRACT

Four mainstream theoretical descriptions of nuclear matter flow are measured against six physical features of nuclei and nuclear heavy-ion collisions. Conventional (one single-determinantal wave function) Time-Dependent Hartree-Fock Theory emerges favorably from the comparison, but fares poorly as a phenomenology. A completely restructured theory, the T.D.-$\mathcal{S}$-H.F., involving many single-determinantal wave functions is proposed by analogy with S-matrix reaction theory. It leads one to place the physical interpretation of the reactions upon time averages of asymptotic channel states of "TDHF Droplets," comprising the translations and periodic TDHF vibrations of isolated integer-nucleon subsystems. In its most naive form (based on small amplitude properties) the theory would consistently describe only the kinematic behavior of "classical" intrinsically dissipative TDHF droplets. But if the periodic solutions of TDHF were to occur only at isolated energies and amplitudes then the theory would describe quantized TDHF droplets with (time-averaged) orthogonal channels, in which periodic solutions play the role of eigenstates in close analogy with the Schrödinger theory.

SUMMARY INTRODUCTION

Those qualitative properties of nuclei, and of their energetic collisions, which seem likely to be 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: perhaps nowhere else in physics will data obtain on the fluid dynamics of the small, finite, self-bound Fermi liquid. The name, Nuclear Fermidynamics, is proposed as an appropriate label for this new realm of physics.

The Principle of Commensurability, which suggests the measurement of the theoretical content of an approach against its expected predictive range and against its intrinsic physical content is set forth and discussed. Several of the current approaches to the nuclear matter flow problem are listed and subjected to a commensurability test.

It is found that the Time-Dependent Hartree-Fock (TDHF) description, alone of all the major theoretical approaches currently in vogue, seems already to incorporate each of the major qualitative

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features within its very concise single mathematical assumption. On the other hand, the Fokker-Planck-type statistical descriptions have so far been the most successful in describing measured results, and the phenomenological applicability of TDHF has been seriously restricted by difficulties of interpretation.

Subsequent discussion focusses on the T.D.-$\mathcal{S}$-H.F. generalization of the conventional single-determinantal method. One of its mechanistic deficiencies (the "Spurious Cross Channel Correlations" introduced whenever one determinant must describe many reaction channels) is identified and corrected by a complete restructuring of the theory from its conventional initial-value form into an S-matrix analogy. The result is a remarkable extension of the conventional single-determinantal initial value problem into a theory with a *separate and distinct* determinant for each possible initial and final reaction channel, which however is still a Hartree-Fock Theory properly so called, since every determinant evolves in time according to its own self-consistent TDHF equation.

The practical requirement that T.D.-$\mathcal{S}$-H.F. one must be able to initialize the time-reversed Hartree-Fock calculation for each final channel state, and the requirement in principle that the measured results predicted by a quantum scattering theory must not depend upon where the (distant) measuring apparatus is located, lead one to characterize the channels by the periodic self-consistent vibrations of separated A_1, A_2 particle systems and the kinematic variables for their relative motion, and to interpret the channel states only in the time-averaged sense.

Thus one circumscribes the apparent physical range of the theory: it describes the reactions between "classical TDHF droplets" whose dynamical content is completely defined by their periodic TDHF vibrations. The simplest of elastic scattering reactions are strongly recommended as objects of numerical computer experimentation, to ascertain to what degree the T.D.-$\mathcal{S}$-H.F. theory in this classical approximation regains the quantal features lost in the conventional TDHF description.

At a more subtle level it is noted that the reaction channels of this classical T.D.-$\mathcal{S}$-H.F. theory are very redundant compared to the complete orthogonal set of Schrödinger functions which they analogize. One result is their non-orthogonality, which in turn leads to some logical strain between two axioms of the theory: the statistical interpretation and the self-consistent TDHF time evolution of each determinantal wave function. The result is that "classical TDHF droplets" on closer look promise to be intrinsically dissipative, "in exhorably sharing their energy ever more widely among the discrete infinity of energy-degenerate vibrations which exist at every finite excitation energy, and defeating thereby both the hope for well-defined asymptotic states, and the possibility for unambiguous time-reversed TDHF calculation from a specific final state.

Finally it is noted that the verification of a single conjecture (namely, that the true periodic solutions of the TDHF equation are *isolated*) would compel the healing of all of these difficulties at once, by altering the set of periodic solutions suitable for characterizing reaction channels from a degenerate continuous

set into a discrete set orthogonal on the time average, and prospectively able to define completely the time-averaged asymptotic properties of the "Quantized" TDHF droplets which such a theory describes.

Thus, one finds that the T.D.-$\mathcal{S}$-H.F. theory describes time-averaged quantum amplitudes whose content depends essentially upon the nature of the periodic solutions to TDHF. If the periodic solutions are isolated then the theory describes Quantized TDHF Droplets which exhibit a dynamical spectrum analogous to the eigenstates of the Schrödinger theory; otherwise, it describes the intrinsically dissipative classical TDHF droplets. Clearly, a rigorous mathematical answer to this question is of the utmost importance. The question is open whether in the latter case, a "Re-quantized" Droplet Theory might still be constructed by the ad hoc addition of some specific quantization assumption to the theory.

This report comprises two major parts as follows:

I. Nuclear Fermidynamics: Physical and Theoretical Commensurability
II. Restructuring TDHF Theory into T.D.-$\mathcal{S}$-H.F.: Classical and Quantal TDHF Droplets.

To fit this paper into the length restriction, we have schematized part II, which at the present stage is of somewhat more technical and specialized interest than part I.

I. NUCLEAR FERMIDYNAMICS: PHYSICAL AND THEORETICAL COMMENSURABILITY

RELEVANT PROPERTIES OF NUCLEI

In this part I, we discuss briefly four 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 four, 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,[1] for a substantial range of low nuclear temperatures.[4]

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.[8-9] We believe, therefore, that it warrants prime consideration in the construction of any theory of nuclear matter flow.[10]

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 hydrodynamical description[11] via equations of the Navier-Stokes type. For such theories deal with intensive variables which are assumed to vary smoothly across the nucleus.

TABLE I: SALIENT FEATURES OF NUCLEAR FERMIDYNAMICS

A.	Four 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 Reponds Self-Consistently to its Own Motion
	4. BCS PAIRED Energy Gap in Particle-Hole Spectrum; Altered Inertial and Dissipation (?) Properties
B.	Two Circumstances of Heavy-Ion Collisions
	1. NON-EQUILIBRIUM <-> Dissipative Suppressed Degrees of Freedom Serve as Dissipative Sink
	2. MASS-DYNAMICAL <-> GLOBAL Matter Flow Substantially Alters Average Field during Process

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[10] is elevated to an exclusive role in the "wall formula" recently recommended by W. J. Swiatecki[14,15] and plays an important part in the various other one-body approaches to dissipation.[16-18]

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[19] and generalized[20] 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.[21-24]

In addition, it has been shown that the inertial tensor for nuclear mass flow will also exhibit Strutinsky-type structure in N, Z, and deformation[25] which can be understood as effecting a locally compressible flow for the nuclear matter.[26] 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.[27] 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 Fermidynamics.

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.

The fourth feature, the Bardeen-Cooper-Schrieffer[29] pairing of nuclei is a long recognized property[30] of low energy nuclear spectra. It is known to imply a moment of inertia smaller than the rigid value,[31] reductions of vibrational inertial parameters,[25] and an energy gap in the spectrum of particle hole excitation of the ground state.[32] Its importance for fission barrier processes has long been recognized,[33] and for dissipation, suspected.[34] It is not yet known how important its effects will be in the Fermidynamics. Indeed, on the grounds that its influence would be quantitative, rather than qualitative, it was omitted from preliminary versions of the present list.[35-36] We here revise this omission.

RELEVANT CIRCUMSTANCES OF NUCLEAR HEAVY-ION COLLISIONS

In addition to the above four 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, 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[37] 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

TABLE II: STRUCTURAL ASPECTS OF COMPLEX MODELS

PHENOMENOLOGICAL:	Does the theory describe the data efficiently?
MECHANISTIC:	Do the processes which are important in the model correspond with the physical processes in the system?
FUNDAMENTAL:	Has the theoretical model been related to well-established basic physical laws?

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 Fermidynamics 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.[14]

THEORETICAL ADEQUACY OF THE MODEL

Besides the question whether a given model adequately incorporates the necessary specific physics, one can also ask whether the resulting description is structurally adequate. In particular we consider the three theoretical structural properties listed in Table II.

COMPARISON AMONG SOME CURRENT THEORIES

In Table III we tabulate four current mainstream theoretical approaches to nuclear heavy-ion collision, Time-Dependent Hartree-Fock,[38-39] Navier-Stokes Hydrodynamics,[40] Fokker-Planck Transport Theory[41] and the One-Body Dissipation Wall Formula,[14] and evaluate them against the six physical features of heavy-ion collisions, and the three general theoretical properties listed. A "Yes" is entered for each feature which a given theory meets; a "No" for each feature which a given theoretical approach omits. Sometimes a Yes or No seems too simple. Then the following remarks attempt further to explain some aspects of Table III.

(A) The TDHF,[42,38-39] as a single-determinantal model of the exact time-dependent Schrödinger problem, would seem to incorporate all the physics of the shell model, including, in its Hartree-Fock-Bogolyubov generalization,[43] the pairing properties. A priori, one would have presumed that TDHF would also incorporate the collisions of particles with the moving wall, which is the essential physics of the Wall Formula for One-Body Dissipation,[14] and, therefore, the dissipation which these collisions are thought to effect. However, recent TDHF calculations[39] of fission yield considerably less dissipation than the One-Body dissipation process for a similar event, raising some question whether this presumption is correct. Thus, the entry, "Yes?"

Conventional TDHF has also been phenomenologically dissapointing in its inability to predict *any specific reaction cross sections whatsoever* (except fusion), and in the fact that the fusion cross sections which it can predict are not unabmiguously fixed but seem to respond to adjustment of the finite range part of the nuclear potential.[44] In summary, as a phenomenology, conventional TDHF so far offers (sometimes) no predictions or offers a vehicle to vary fundamental parameters in such a way as to extract a broad variety of predictions,[45] which however may or may not adhere essentially to the physics of TDHF. Thus, "No?". Mechanistically, TDHF appropriately describes nucleonic motion of long mean free path; in complex reactions, however, it seriously mistreats multi-channel situations, as discussed in part II below. Thus, "Yes, but*".

(B) Navier-Stokes Hydrodynamics[40] as the dynamical generalization of the static liquid drop model of nuclei is a most natural candidate for describing Fermidynamics. However it seems essentially related to the short mean free path property of water-like liquids,[13] and therefore most unlikely to describe the small, finite, paired Fermi system. This deficiency makes its mechanistically unsound, and, defeats in the nuclear case hydrodynamics' demonstrated connection[13] for other liquids with more fundamental physics.

(C) The Fokker-Planck Transport theory description[41] of energy, charge, and mass equilibrization between two fragments in deep inelastic contact might describe systems with various mean free paths or flow properties by incorporating their respective effects into its phenomenological transport coefficients. The difficulty of tracing these coefficients quantitatively to their mechanistic causes seems a fair basis for some restraint upon the optimism which the phenomenological success of this approach might otherwise sustain. Therefore the entries, "?".

(D) The Wall Formula for One-Body Dissipation[14] (which is an extension of the piston model[16] to the complete 4π surface' 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 upon the Fermi particles (thus, "Yes?" in Table III). Also, its recent generalization to wave mechanical motions of the particles in the box[18] and the previously established connections[28] between the degeneracies of such solutions and the Strutinsky generalized shells opens the possibility (Yes?) that Finite-A effects may find a natural place in the one-body Wall Formula. Since the Wall Formula is narrowly aimed at dissipation it seems to involve no particular assumptions about binding, matter flow, or pairing. Therefore we leave for these items blank. The Wall Formula has been phenomenologically successful in describing the fission fragment kinetic energies. But at the fundamental level it clearly suffers from oversimplification: without ad hoc alteration it violates Gallilean invariance, conservation of momentum, and the Pauli exclusion principle for the rebounding particles.

TABLE III: PHYSICAL AND THEORETICAL PROPERTIES OF SEVERAL THEORIES

	Property: \ Theory:	*CONVENTIONAL TIME-DEPENDENT HARTREE-FOCK THEORY*	*NAVIER-STOKES HYDRODYNAMICS*	*FOKKER-PLANCK TRANSPORT THEORY (including Window Formula)*	*ONE-BODY DISSIPATION: WALL FORMULA*
PHYSICAL	SMALL-FERMI ($\lambda > R$)	Yes	No	No?	Yes?
	FINITE-A (Generalized Shells)	Yes	No	No?	Yes?
	LIQUID (Self-bound)	Yes	Yes	No	----
	BCS PAIRED	Yes (TDHFB)	No	No?	----
	GLOBAL, MASS-DYNAMICAL	Yes	Yes	No	----
	NON-EQUILIBRIUM DISSIPATIVE	Yes(?)	Yes	Yes	Yes
STRUCTURAL	PHENOMENOLOGICAL	No?	?	Yes	Yes
	MECHANISTIC	Yes, but*	No	?	Yes
	FUNDAMENTAL	Yes?	No	?	No

*See Spurious Cross Channel Correlations in part II, and Refs. 35, 36, 46.

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, yields no assurance that the resulting description will adequately describe observed nuclear data. Nevertheless, we feel that TDHF should be of great interest in and of itself, and especially because of the very economy of its assumptions, as a theorists' theory, whence to learn how to look at the problems of the Fermidynamics. It is for this reason, rather than from an expectation of imminent successful confrontation between TDHF and observed data, that we devote some considerable discussion to this model below. And if, in the process, the phenomenology can be improved, then all the better.

Also, it need hardly be said that Table III is itself a time-dependent function of one's understanding of the problem.

THE PRINCIPLE OF COMMENSURABILITY IN THE ASSESSMENT OF DESCRIPTIONS OF COMPLICATED PHENOMENA

We note that one can formulate the present approach 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,[35,36,47] 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 focusing 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 properties, but whose *physical* implications are not immediately transparent.

II. RESTRUCTURING TDHF THEORY INTO T.D.-$\mathcal{J}$-H.F.: CLASSICAL AND QUANTUM DROPLETS

[For brevity, this section is presented in lecture-note outline form. Some elaboration will be found in Refs. 35, 36, and 46.]

CONVENTIONAL TDHF[38,39,42]

1. Replaces exact $\Psi \rightarrow \Phi$, a single determinant
2. propagates in time via nonlinear TDHF Equation, from
3. the initial value, $\Phi(t)\big|_{t-t_i} = \Phi_0$.
4. TDHF is approximate:
   a) Initial single-determinant is inexact and inflexible.[47]
   b) Time propagation is approximate.[48]
   c) Post-breakup determinant is too simple and, heretofore, uninterpretable.

SPURIOUS CROSS CHANNEL CORRELATIONS[35,36]

1. In late stages of the reaction many channels must be described. But,
2. a single-determinant can at most describe some crude average channel, and therefore, such a determinant
3. cannot be self-consistent for *any* specific channel.

TDHF S-MATRIX ANALOGY

Consider $\mathcal{S}_{fi}$, the TDHF analog of the exact S-Matrix

$$\langle \Psi_f^{(-)} | \Psi_i^{(+)} \rangle = S_{fi}, \tag{1}$$

obtained by replacing the exact Ψ_g by Φ_g, the TDHF solutions initialized with conditions g,

$$\mathcal{S}_{fi} = \langle \Phi_f^{(-)} | \Phi_i^{(+)} \rangle. \tag{2}$$

Evidently $\mathcal{S}_{fi}$ may vary rapidly with time. Then construct

$$\bar{\mathcal{S}}_{fi} = \frac{1}{T_2 - T_1} \int_{T_1}^{T_2} \langle \Phi_f^{(-)}(t') | \Phi_i^{(+)}(t') \rangle \, dt' \tag{3}$$

by time averaging $\mathcal{S}_{fi}$ over the interaction inverval.[49] Then have a description in which $\Phi_i(t)$ at late times is replaced by

$$\Xi(t) \underset{t\to\infty}{\Rightarrow} \sum_f \hat{\mathcal{S}}_{fi} \, \Phi_f(t) \tag{4}$$

where $\hat{}$ indicates $\bar{\mathcal{S}}$ normalized with respect to initial state. Ξ involves

a) one separate conventional TDHF calculation for each channel, f.
b) no spurious cross channel correlations.

DEFINITION OF CHANNELS IN T.D.-$\mathcal{S}$-H.F.

For each channel, f, demand the ability

a) to initialize unambiguously TDHF propagation of Φ_f, (the Initialization Requirement) (5a)
b) to measure physical information on fragments independent of the (asymptotic) location of the apparatus (the Asymptoticity Requirement) (5b)

Then find that

c) intrinsic states must be (stable) stationary H.F. solutions, or (if time average is considered) periodic TDHF solutions. (N.B., *almost periodic* solutions do *not* suffice because the initialization process becomes impractical.) (6)

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

$$\{f\} = (A_1, S_1, A_2, S_2, \vec{R}_f / |R_f| \vec{V}_f, t_f; \varepsilon_{\lambda_1}, \phi_{\lambda_1}, \varepsilon_{\lambda_2}, \phi_{\lambda_2}). \tag{7}$$

This set of labels symbolizes:

1. A single $(A_1+A_2) \times (A_1+A_2)$ determinant constructed by antisymmetrizing;
2. an $(A_1 \times A_2)$ determinant describing the S_1 the stable 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 (stable) 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 periodically, with period τ_λ and with amplitude ε_λ, and
   d) at time $t = t_f$ is at a particular phase of its oscillation, denoted by ϕ_λ.

In addition,

5. the time-dependent complex C-number phase of the wave function[49] is chosen according to the constant $-\langle \mathcal{H} \rangle$ prescription[50] to be exp $- i\langle H \rangle t/\hbar$.

FUNDAMENTAL AXIOMS OF T.D.-$\mathcal{H}$-H.F.

A) The statistical interpretation of quantum mechanics holds for TDHF solutions, Φ_g.

B) Self-consistent TDHF propagation describes the time evolution of any determinant:

$$\mathcal{H}[\Phi(t)]\Phi(t) = i\hbar\,\dot{\Phi}(t). \tag{8}$$

Axiom (A) justifies interpretation of $\langle \Phi_f^{(-)}(t') | \Phi_i^{(+)}(t') \rangle$ in Eq. (2) as the probability amplitude that Φ_i would be found at t' to be the state Φ_f, which would subsequently evolve in time into the specific channel state $\{f\}$.

However, consistent application of axiom (A) also implies that (time-averaged) non-orthogonality of channel functions

$$O_{ff'}^{(t)} = \lim_{\sigma \to \infty} (2\sigma)^{-1} \int_{t-\sigma}^{t+\sigma} \langle \Phi_f^{(-)}(t') | \Phi_{f'}^{(-)}(t') \rangle \, dt', \qquad (t \gg \sigma \gg T_2) \tag{9}$$

$$\neq (\{f\} - \{f'\}), \tag{10}$$

should be interpreted to indicate transitions among channel states; i.e., continued alteration of the population of various channels, even at asymptotically late times—in violation of the asymptoticity requirement (5b).

SMALL AMPLITUDE VIBRATIONS: CLASSICAL TDHF DROPLETS

If the Small Amplitude self-consistent TDHF vibrations[51] are adopted as the periodic solutions labelled in (7), then

a) at every excitation energy, these periodic solutions exhibit a discretely infinite degeneracy. (11a)
b) the overlap function, (9), indicates (time-averaged) non-orthogonality for the channels. (11b)

Because of the fact that the vibrational energies in this case are continuous we refer to such systems as "classical" TDHF droplets.

CLASSICAL TDHF DROPLETS ARE INTRINSICALLY DISSIPATIVE

Then the only asymptotically constant state (if any existed) of classical droplets (12) would have to be some "thermalized" internal equilibrium state characterized solely by the excitation energy, E^*. Therefore, we say that classical TDHF droplets are "intrinsically dissipative." Their theory can describe at most mass transfer and the reaction kinematics of relative motion, but no specific information about the internal states of the final droplets, except for excitation energy, E^*.

IF PERIODIC SOLUTIONS ARE ISOLATED, TDHF DROPLETS ARE QUANTIZED AND CHANNELS ARE ORTHOGONAL

A qualitatively different situation prevails if the periodic TDHF solutions exist only at isolated values of the period and the amplitude (and therefore with discrete energy) rather than in continuous families such as those describing small amplitudes. Then in each periodic channel solution, $\{f'\}$, one fragment wave function is of the form

$$\Phi_{f'} = \{\exp - i\, E_{f'}\, t/\hbar\}\{ \sum_{p\ \text{integral}} \phi^{p}_{f'}(\vec{r}-\vec{v}_{f'}, t)\, \exp\, i\, p\, \omega_{f'}, t\} \qquad (12)$$

with a discrete total energy, E_f, and a time-averaged overlap integral with another channel $\{f\}$, given by (10):

$$O_{ff'} = \lim_{\upsilon\to\infty} (2\upsilon)^{-1} \int dt' \langle \phi^{q}_{f}(\vec{r}-\vec{v}_{f}t) \,|\, \phi^{p}_{f'}(\vec{r}-\vec{v}_{f'}t)\rangle \times \{\exp - it(E_{f'}-E_{f}+q\hbar\omega_{f}-p\hbar\omega_{f})/\hbar\} \qquad (13)$$

which vanishes unless

$$\vec{v}_{f} = \vec{v}_{f'}, \text{ and} \qquad (14)$$

$$E_{f'} - p\hbar\omega_{f'} = E_{f} - q\hbar\omega_{f}. \qquad (15)$$

Since, apart from an accidental degeneracy of the discrete energies, these conditions can be met only by $\{f\} \equiv \{f'\}$, we obtain the channel orthogonality condition

$$O_{ff'} = \delta(\{f\} - \{f'\}). \qquad (16)$$

Thus, isolated periodic TDHF solutions imply

a) *Quantized* TDHF droplets with discrete vibrational energies.
b) Asymptotic channels which are
   i) (time-averaged) orthogonal, and
   ii) propagate without changing in time (on the average) according to *both* T.D.-$\mathscr{A}$-H.F. axioms (A) and (B).
c) A T.D.-$\mathscr{A}$-H.F. reaction theory exhibiting a structure fully analogous to the Schrödinger theory, in which periodic solutions play the role of eigensolutions.

CREATE, IF NECESSARY, A THIRD AXIOM TO ISOLATE CHANNEL SOLUTIONS?

It is obvious that the mathematical nature of the TDHF periodic solutions is crucial to interpreting the T.D.-$\mathscr{A}$-H.F. reaction theory and that the mathematical property of isolation of the peri-

odic TDHF solutions, would impose most naturally upon TDHF a full analogy with the exact Schrödinger theory.

But if the periodic solutions are in fact not isolated, then the question would arise whether a suitable third axiom could be found which would select a discrete subset of periodic solutions as the appropriate set of channel states. These channels ought to conform to the initialization and asymptoticity requirements (5), meet the orthogonality condition (16), and suffice to characterize exhaustively any post-reaction state (4). Whether such an axiom can be found is an open question.

RECAPITULATION

A broad-based comparison of the physical content of several theories of Fermidynamics identifies TDHF as especially relevant to the problem even though it is axiomatically terse. One mechanistic deficiency (spurious cross channel correlation) is obviated by restructuring the theory from a single wave function theory into a multi-wave function theory, with one single-determinantal wave function for each reaction channel. Depending upon the nature of the periodic solutions to the TDHF problem the resulting theory can offer a restricted kinematic description of reactions among classical TDHF droplets or a description of reactions of quantized TDHF droplets substantially analogous to the Schrödinger theory. Whether in the former case the droplets might be "requantized" by an additional axiom is an open question.

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