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SINGLE DETERMINANTAL REACTION THEORY AS A SCHRÖDINGER ANALOG: THE TIME-DEPENDENT $\mathcal{S}$-MATRIX HARTREE-FOCK METHOD

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ABSTRACT

We suggest that the TDHF method be viewed, not as an approximation to but as a model of the exact Schrödinger system; that is, as a gedanken many-body experiment whose analysis with digital computers provides data worthy in itself of theoretical study. From such a viewpoint we focus our attention on the structural analogies of the TDHF system with the exact theory rather than upon its quantitative equivalence, and we study the TDHF many-body system as a challenge of its own which, although much simpler than the realistic problem, may still offer complexity enough to educate theorists in our present state of knowledge.

In this spirit, the TDHF description of continuum reactions can be restructured from an initial-value problem into a form analogous to the S-matrix version of the Schrödinger theory. The resulting TD-$\mathscr{S}$-HF theory involves only self-consistent single determinantal solutions of the TDHF equations and invokes time averaging to obtain a consistent interpretation of the TDHF analogs of quantities which are constant in the exact theory, such as the S-matrix and the asymptotic reaction channel characteristics.

Periodic solutions then play the role of stationary eigenstates in the construction of suitable asymptotic reaction channels. If these periodic channel states occur only at discrete energies, then the resulting channels are mutually orthogonal (on the time average) and the theory exhibits a structure fully analogous to the exact theory. In certain special cases where the periodic solutions are known to occur as an energy continuum, the requirement that the periodicity of the channel solutions be gauge invariant provides a natural requantization condition which (suggestively) turns out to be identical with the Bohr-Sommerfeld quantization rule.

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I. INTRODUCTION

Since the TDHF method [1] was first computerized as a nuclear model [2], studies based upon its numerical calculation have burgeoned [3]. As an approximation to the Schrödinger equation, the precise limits of its applicable physical range have remained largely unspecified. As a model of the Schrödinger system, stemming from the same variational principle with only the single additional restriction to single determinants, deeper questions arise regarding the very interpretation of the TDHF solution for the reaction process: In what sense is it at all a proper Schrödinger wave function? Can it describe amplitudes for reactions leading to specific internal states of the final ejectiles, or does it contain only information averaged (in what manner?) over many final states? Or more generally, what is the precise effect on the physical content and the mathematical structure of the theory of the additional restriction to single determinants?

In addition, certain fundamental difficulties in the interpretation of solutions calculated to describe reactions remain unsolved and appear insoluble within the initial value TDHF framework. For example, conventional TDHF predicts an amplitude for the internal characteristics of the ejectile which depends upon the location of the measuring apparatus (non-asymptoticity). In addition, the mean field so essential to the whole method is structurally incapable of describing adequately the full kinematic range of final reaction channels (spurious cross-channel correlation).

In this paper we review certain aspects of the $\mathcal{S}$-matrix approach to these questions [6], and report new developments based on the nature of the periodic TDHF solutions to certain model problems [7]. We show that a consistent description of quantum reaction amplitudes, which is structurally fully analogous to the Schrödinger theory, can be built upon (the whole set of) self-consistent TDHF solutions, provided that the asymptotic channel states employ gauge invariant periodic solutions as the analogs of Schrödinger eigenstates and the physical implications of the theory are interpreted on a time-averaged basis. The corollary implication for nuclear structure theory, that gauge invariant periodic TDHF solutions are the appropriate "TDHF-eigensolutions" for describing bound states in the time-dependent framework is noted [7].

II. COMMON VARIATIONAL ORIGINS OF TDHF AND SCHRÖDINGER THEORIES

The Variational Principle

$$\delta I = \delta \int_{t_1}^{t_2} \langle\Psi|(H - i\hbar\partial/\partial t)|\Psi\rangle dt' = 0 \qquad (1)$$

implies the exact nonrelativistic time-dependent Schrödinger equation [8]. If the wave function Ψ is required to be a single determinant, the same principle yields the unique "Constant-$\langle\mathcal{H}\rangle$" time-dependent Hartree-Fock equation [9]. Since the origins of the TDHF model and those of the Schrödinger theory lie so close, a close structural parallel between them is reasonably to be expected. It is that analogy which is discussed in this paper.

III. SIX ASPECTS OF THE TDHF-SCHRÖDINGER PARALLELISM

The discussion will consider six interrelated aspects of the TDHF-Schrödinger parallelism, as follows;

(a) the Asymptoticity of the reaction theory--whether its predicted results depend upon the precise location of the distant measuring apparatus or not;

(b) the Periodicity of solutions for isolated system;

(c) Time-Averaging, under which periodic solutions become characterized by constants and allowed a role analogous to the stationary state eigensolutions of the exact theory;

(d) Asymptotic Channel Orthogonality, which does not prevail among the solutions of the nonlinear TDHF theory, but which by time averaging can be regained for asymptotic channels describing periodically vibrating droplets, provided that their energies are discrete rather than continuous;

(e) Requantization, by which certain periodic solutions of discrete energy can be selected from a continuum of periodic solutions to serve the role analogous with that of the channel eigenfunctions of the exact theory;

(f) Gauge Invariance--the property of the exact eigensolutions which offers a natural basis for the requantization of the continuous periodic TDHF spectrum (and which leads, remarkably, for certain model problem to the same quantized states as the Bohr-Sommerfeld quantization rules would select).

IV. ASYMPTOTICITY IN A REACTION THEORY

In the exact Schrödinger theory, the wave function describing the system for times long after the collision process can be expanded upon a complete mutually orthogonal basis of channel states, constructed from the eigenstates of every possible pair of fragments, and the functions describing their relative motion. It follows that the probability of measuring a certain value for any internal physical property of an ejected fragment is predicted not to depend upon the precise location of the measuring apparatus with respect to the collision volume, provided only that it is sufficiently distant to guarantee that the interactions between the fragments vanish. This independence of the predictive content of a reaction theory of the precise location of the measurement, we refer to as the "Asymptoticity" property of the theory. Clearly the Schrödinger theory exhibits this property.

V. INITIAL VALUE TDHF THEORY LACKS ASYMPTOTICITY

Asymptoticity is not a general property of the conventional initial value TDHF theory, because of the fact that the self-consistency condition leads to a time evolution operator (the Hartree-Fock "Hamiltonian", $\mathcal{H}$) which is a functional of its solution, and therefore continues to be time-dependent, even long after the collision. Needless to say, this non-asymptoticity of TDHF lies at the root of the difficulties of the precise interpretation of the physical implications of conventional initial-value TDHF descriptions of complex reactions. As a result, only a few "trajectory" characteristics, which remain constant once the fragments separate have been extracted from the numerical TDHF studies of nuclear system, in pale contrast with the rich detail which the corresponding Schrödinger solution would, in principle, yield. For what useful meaning could be attributed to theoretically predicted reaction amplitudes which vary with the location of the counting apparatus?

Thus, although the expectation has frequently been expressed that some such an unambiguous interpretation would be found for the late time wave functions of conventional intitial-value TDHF theory, only one report of an explicit attempt is known to the present authors [10]. The result was that the expansion coefficients remained time-dependent indefinitely.

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

The TD-$\mathcal{S}$-HF approach to the single determinantal reaction theory [6] has been evolved by requiring the closest possible analogy between the self-consistent TDHF description and the exact Schrödinger theory. In particular, the general requirement has been imposed at every stage that the TD-$\mathcal{S}$-HF must reduce identically to the Schrödinger description in case the exact solution happens to be a single determinant.

The S-matrix form of the Schrödinger reaction theory for localized wave packets has been chosen as the model to be imitated. Thus, the symmetry in time which that theory displays is retained, together with the close parallel implied between possible initial and final reaction channel states.

Two rigid conditions imposed upon the theory have been set as axioms. The first specifies the precise meaning of TDHF self-consistency, by requiring that every wave function allowed in the theory must be a single determinant and must propagate in time according to the self-consistent TDHF equation,

Axiom (A): $$\mathcal{H}[\Phi] \cdot \Phi = i\hbar\dot{\Phi}. \tag{2}$$

The second requires every wave function allowed in the theory to be subject to the statistical interpretation of quantum mechanics, in the sense that the spatial integral,

Axiom (B): $$a_{fi} = \langle\Phi_f|\Phi_i\rangle, \tag{3}$$

specifies the probability amplitude that a system described by Φ_i will under physical measurement exhibit the characteristics of the system described by Φ_f.

Without Axiom (A) a theory is not a self-consistent TDHF theory; lacking Axiom (B) the solutions are not Schrödinger wave functions, properly so called. It is hard to imagine any objection to either; the question is rather whether they can be sustained without preventing the construction of a theory reasonably analogous to the Schrödinger theory.

As its name implies, the TD-$\mathcal{S}$-HF reaction theory casts the Schrödinger S-matrix in a prominent role. Indeed, the S-matrix analog,

$$\bar{\mathcal{S}}_{fi} = (T_2-T_1)^{-1} \int_{T_1}^{T_2} \langle\Phi_f(\vec{x},t')|\Phi_i(\vec{x},t')\rangle dt', \tag{4}$$

describes the transition probability from an initial to a final self-consistent TDHF reaction channel. In ref. [6] the form (2) for $\bar{\mathcal{S}}$ is obtained heuristically by analogy with the exact Schrodinger theory in such a way that it reduces exactly to the S-matrix when the single determinantal solutions, Φ, are also solutions of the exact Schrödinger equation. In addition, the palpable physical error introduced by the spurious cross channel correlations of the conventional Hartree-Fock description during the postbreakup phase, when the description of several channels is imposed upon the single determinant, is eliminated from the theory.

VII. ASYMPTOTICITY AND PERIODICITY

Under the ansatz (4) the single determinantal description is released from the narrow constraints of the initial value formulation. One result is a freedom, and a need, to select reaction "channels" suitable for the physical description required. Then by selecting the reaction channels so as to assure that the physical properties of the emergent droplets remain constant in time, one achieves the first step towards guaranteeing asymptoticity for the new theory.

This condition requires that a reaction channel wave function must describe stationary TDHF states of the emergent droplets. Or, if periodic TDHF states are allowed as channel states, then their physical properties can be considered as constant if interpreted on a time-averaged basis.

VIII. INITIALIZABILITY AS A NECESSARY CHANNEL PROPERTY

The construction (4) of the $\bar{\mathcal{S}}_{fi}$ reaction requires that one solution $\Phi_f(\vec{x},t)$ correspond with each channel, specified by a set of labels {f}. Together with the TDHF self-consistency axiom, eq. (2), it imposes the requirement of "initializability" upon each channel: the labels for any channel {g} must be precisely those required to initialize a unique TDHF calculation for the solution, Φ_g. In ref. [6] this selection is discussed in some detail with the conclusion that the labels,

$$\{f\} = \{(A_f^{(1)},\{\lambda_f^{(1)}\},\vec{v}_f^{(1)});\ (A_f^{(2)},\{\lambda_f^{(2)}\},\vec{v}_f^{(2)});\ R_f/|R_f|,t_f\}, \tag{5}$$

suffice to specify the state of two subdeterminants #1 and #2 located at t_f at some large standard separation distance $|R_f|$, moving with velocities $\vec{v}_f^{(1)}$ and $\vec{v}_f^{(2)}$ (related by the requirement of zero center of mass momentum) and comprising subdeterminantal fragments of $A_f^{(1)}$, $A_f^{(2)}$ nucleons (or $N_f^{(1)}$, $Z_f^{(1)}$, $N_f^{(2)}$, $Z_f^{(2)}$ neutrons and protons, respectively), whose internal states at time t_f are defined by two sets of parameters, $\{\lambda_f^{(1)}\}$, $\{\lambda_f^{(2)}\}$. E.g., for the periodic internal states, $\{\lambda_f^{(1)}\}$ would identify the particular periodic state and specify the point in its period at which it is found at the initializing time $t = t_f$.

IX. TIME AVERAGING IN THE TD-$\mathscr{S}$-HF THEORY

The use of periodic solutions to play the role of the exact eigenstates for the description of TDHF droplets in the asymptotic channel states, implies that their asymptotically constant physical characeteristics must be characterized by time averages (over the period) of physical operators. We note that also in the definition of $\mathscr{S}$, the time average defined by eq. (2) was a consequence of the fact [6] that the overlap of two TDHF solutions, in contrast with the S-matrix overlap between exact solutions, is not constant in time. Thus (2) specifies that the reaction amplitude is to be obtained by time averaging over the whole interaction interval.

X. TIME AVERAGING AND ASYMPTOTIC CHANNEL ORTHOGONALITY

Still a third cause for a time averaged interpretation arises now in connection with the asymptoticity of the channel states built upon the periodic TDHF solutions proposed to describe the droplets--this time stemming from the mutual non-orthogonality of such solutions. Here again we deal with a deviation of the TDHF from the exact theory which arises from the self-consistency condition: the eigenstates of the exact linear Schrödinger Hamiltonian form a complete, orthogonal, linearly superposable set, while the TDHF "Hamiltonian" generates a set of stationary (and periodic) solutions which are not mutually orthogonal and which cannot be superposed to form arbitrary solutions, because of the nonlinearity of the TDHF equations they obey.

As a result of the non-orthogonality of the TDHF solutions, overlap amplitudes between distinct final channel functions, such as

$$a_{gf} = \langle \Phi_g(\vec{x},t) | \Phi_f(\vec{x},t) \rangle, \tag{6}$$

do not automatically vanish. It follows that under the statistical interpretation of quantum mechanical amplitudes (Axiom B in eq. (3)), the statement that a system is described by the solution, Φ_f, must also assert with a probability, a_{gf}, that a measurement would show it to have the properties of channel {g}. Then the reaction amplitudes $\bar{\mathcal{S}}_{fi}$, would not correspond one-to-one with the theoretical predictions for measured properties, {f}.

This difficulty also is resolved by the assumption that the amplitudes (3) must be interpreted not instantaneously, but on a time averaged basis. Then, not a_{gf} of (6), but its time average value,

$$\overline{a_{gf}} = (2\tau)^{-1} \int_{t-\tau}^{t+\tau} \langle\Phi_g(\vec{x},t')|\Phi_f(\vec{x},t')\rangle dt' \qquad (7)$$

is to be interpreted as the amplitude that a system described by the solution, Φ_f, will be measured to have the physical properties of channel {g}. (In eq. (7), τ must be taken large enough for a_{gf} to be independent of the interval, τ; in the asymptotic region, this is always possible.) Then, as was shown in ref. [6], the time averaged overlaps between distinct asymptotic channels all vanish,

$$\overline{a_{gf}} = 0 \qquad \{g\} \neq \{f\} \qquad (8)$$

if only the energies of the periodic channel solutions are discrete and nondegenerate.

Thus, for channel states built upon a discrete nondegenerate set of periodic TDHF solutions, the time averaged channel orthogonality property (8) prevails. Then the one-to-one correspondence between the reaction amplitudes and the theoretically predicted values of the (now time averaged) physical measurements which prevails in the exact reaction theory is retrieved for the TD-$\mathcal{S}$-HF theory.

XI. REQUANTIZATION AND GAUGE INVARIANCE

Although it is not known whether the periodic TDHF solutions for isolated TDHF droplets occur always with a continuous range of energies, Kan, et al. [7] have recently studied special cases for which this situation prevails. (Note that the harmonic solutions obtained in TDHF in the small amplitude approximation [11] do not suffice as examples to this point, since one does not know whether or not the corresponding exact TDHF solutions are truly periodic, obeying for all t the identity,

$$\Phi_p(\vec{x},t+T) = \Phi_p(\vec{x},t), \qquad (9)$$

or merely obey it approximately over some limited time interval.) Kan's work therefore forces one to deal with the Requantization process discussed in ref. [6], by which some set of solutions discrete in energy is selected from the continuous spectrum of periodic TDHF solutions to serve as reaction channel wave functions; or else to conclude that the single determinantal reaction theory, since it would then lack reaction channel orthogonaltiy, and therefore could not consistently predict physical measurements in one-to-one correspondence with the reaction channel amplitudes characterizing the reaction process, was of an essentially different character, structurally, from the exact theory--an "intrinsically dissipative" trajectory theory, in the terminology of ref. [6].

We again proceed by analogy with the Schrödinger theory, this time utilizing the gauge invariance of its physical content. Then, remarkably, one finds that the requirement that the TDHF solutions behave like the exact stationary eigenstates, and particularly that they be invariant under gauge transformations, leads to a unique and unambiguous selection of a discrete set of gauge invariant periodic functions as suitable eigenstate analogs.

One can view this process as a requantization procedure dictated by the gauge properties. Alternatively, one might take the view that, in spite of the fact that the periodic spectrum of TDHF solutions may in some cases be continuous, nevertheless the periodic solutions capable of playing the role of eigenstates, especially as regards gauge transformation properties, occur only as a discrete set.

XII. GAUGE INVARIANCE OF THE TIME-DEPENDENT SCHRÖDINGER THEORY

Consider the Schrödinger system characterized by the (time-independent) Hamiltonian, H, and the set of time-dependent descriptions specified by the gauge transformed Hamiltonian operators, $\hat{H}$, of the form

$$H \rightarrow \hat{H} = H + \beta(t) \tag{10}$$

where $\beta(t)$ is an arbitrary space and momentum independent function of time.

Then the physical content of each of the transformed descriptions is exhausted by the matrices of all the possible physical observables, $\mathcal{O}(\vec{x},\vec{p})$. Moreover, every such matrix of the system, H, is identical with the corresponding matrix of the system, $\hat{H}$, element by element,

$$\langle\hat{\Psi}_i|\mathcal{O}(\vec{x},\vec{p})|\hat{\Psi}_j\rangle \equiv \langle\Psi_i(\vec{x},t)|\mathcal{O}(\vec{x},\vec{p})|\Psi_j(\vec{x},t)\rangle. \tag{11}$$

Equation (11) follows from the fact that a change in $\beta(t)$ alters each of the solutions only by a time-dependent complex phase factor which is the same for every solution, Ψ_i. (In passing, we contrast this universal phase factor with the state-dependent phase factors implied by the TDHF variational principle, as discussed in ref. [9].)

Note that among the physical observables, there must occur the energy operator, given by the Hamiltonian, $H(\vec{x},\vec{p})$. Obviously, under the transformation (10) the diagonal matrix elements of H (but not the off-diagonal elements) in (11) all shift by the amount, $\beta(t)$. Since, in fact, only energy differences are physically observed, and not absolute values of the energy, such a shift does not affect the physical content of the theory.

XIII. GAUGE INVARIANCE OF EIGENSTATES

Then consider the time-dependent Schrödinger solution initiated at $t = t_0$ as an eigenfunction, $\psi_\lambda(\vec{x})$, such that,

$$H\,\psi_\lambda(\vec{x}) = E_\lambda\,\psi_\lambda(\vec{x}). \qquad (12)$$

(We use the Greek subscript to distinguish the eigenfunction case from the more general initial conditions denoted by Latin subscripts.) Such a time-dependent solution is, for arbitrary gauge, $\beta(t)$ in (10), of the form,

$$\psi_\lambda(\vec{x},t) = \psi_\lambda(\vec{x})\{\exp - (i/\hbar)[E_\lambda(t-t_0) + \int_{t_0}^{t} \beta(t')dt']\} \qquad (13)$$

$$= \psi_\lambda(\vec{x})\{\exp - (i/\hbar)\int_{t_0}^{t} \langle\Psi_\lambda|\hat{H}(t')\Psi_\lambda\rangle dt'\}. \qquad (14)$$

The latter form in (14) is written to emphasize the fact that under gauge transformation, (10), only the phase factor is altered, while the stationary state remains invariant. By analogy with the stationary eigenfunctions, then, we shall insist that the periodic channel solutions of TDHF must also be invariant under arbitrary gauge transformation.

XIV. "TD-$\mathcal{H}$-HF EIGENSOLUTIONS": PERIODIC STATES AS GAUGE ANALOGS OF THE EXACT STATIONARY EIGENSTATES

In the Hartree-Fock case, consider the "Constant-$\langle\mathcal{H}\rangle$" solutions defined by the equation,

$$\mathcal{H}[\Phi]\cdot\Phi = \{\mathcal{H}^o[\Phi] + \langle\Phi|H - \mathcal{H}^o[\Phi]|\Phi\rangle\}\cdot\Phi = i\hbar\dot{\Phi}, \qquad (15)$$

and a specified initial-value determinant. The TDHF "Hamiltonian", $\mathcal{H}$, of eq. (14) is uniquely prescribed [9] by the variational principle (1). Then $\mathcal{H}^o$ may be the conventional self-consistent Hartree-Fock Hamiltonian, or that Hamiltonian augmented by any arbitrary additive function of time only. Now consider the effect upon a periodic solution, $\Phi_p(\vec{x},t)$, of (15) of a gauge transformation (9). The new solution is related to the old by a phase factor,

$$\hat{\Phi}(\vec{x},t) = \Phi_p(\vec{x},t)\{\exp - (i/\hbar) \int_{t_0}^{t} \beta(t')dt'\}. \tag{16}$$

Obviously, $\hat{\Phi}$ need not be periodic even when Φ_p is periodic. Therefore, it is not possible for periodicity in general to be a guage invariant property.

Then to sustain the analogy between the exact theory and TDHF under gauge invariance, we must seek channel solutions in the form of a product of a periodic function and a phase factor determined by H alone; i.e.,

$$\Phi(\vec{x},t) = \Phi_p(\vec{x},t)\{\exp - (i/\hbar) \int_{t_0}^{t} \langle H(t')\rangle dt'\} \tag{17}$$

where Φ_p is a periodic function satisfying (9). A function of the form (17) will transform under the gauge transformatin of H in preicsely the same way as the exact solution (14), and the periodic solution, $\Phi_p(\vec{x},t)$ is precisely the anlogy of the stationary eigenstate, $\psi_\lambda(\vec{x})$.

XV. GAUGE INVARIANT TDHF EQUATION

Of course, the function (17) must satisfy the (unique!) TDHF equation (14) implied by the variational principle (1). Then the periodic factor, Φ_p, of (17) satisfies the following equation,

$$\{\mathcal{H}[\Phi_p] - \langle\Phi_p|\mathcal{H}|\Phi_p\rangle\} \cdot \Phi_p = i\hbar\dot{\Phi}_p. \tag{18}$$

We refer to (18) as the gauge invariant TDHF equation, since it is manifestly unaffected by any transformation of the form (10).

XVI. CONTINUA OF PERIODIC TDHF SOLUTIONS: GAUGE REQUANTIZATION

For certain model problems, Kan, et al. [7] show that eq. (15) exhibits, for time-independent H, a continuous set of periodic solutions. But among such a continuum, only those solutions whose energy is related to the period, T, by the equality,

$$E = \langle\Phi_p|H|\Phi_p\rangle = 2N\pi\hbar/T, \tag{19}$$

are of the form (17) with a periodic factor which satisfies the gauge invariant TDHF equation (18). Then (19) selects a discrete subset of the periodic continuum, for which the space-dependent periodic factor, Φ_p, is invariant under the gauge transformation (10), exactly as are the eigenstates of the exact Hamiltonian.

Thus, condition (19) offers a natural basis for the requantization of the continuum of periodic TDHF solutions into a discrete set of TDHF eigenfunctions. It selects those periodic states which remain periodic, just as the eigenstates remain stationary, under an arbitrary gauge transformation. In turn, the TD-$\mathscr{S}$-HF channel wave functions are all initializable in terms of specific periodic states, independent of the choice of gauge. And their discreteness in energy guarantees also the mutual (time averaged) orthogonality property (8) for them, providing thereby under the statistical interpretation of the wave functions, a consistent one-to-one correspondence between the reaction amplitudes and the theoretical predictions of the internal droplet properties.

Alternatively, one could have sought in the first place as suitable analogs of the stationary eigenstates only those solutions whose periodity is a gauge invariant periodic function, like the stationarity of the eigenstates. Then one would at the outset have recognized only the discrete periodic spectrum of (18) as acceptable channel states, rather than the continuous set of periodic solutions of (15).

We note that Kan, et al., [7] have also demonstrated the equivalence of the condition (19) with the Bohr-Sommerfeld quantization condition.

XV. "TDHF EIGENSTATES"

The gauge invariant periodic solutions offer a discrete spectrum of TDHF states which share the gauge transformation properties of exact time-dependent eigenstate solutions. These states are therefore natural objects to describe the large amplitude TDHF analogs of the Schrödinger eigenstates within the time-dependent framework.

Indeed, by numerical calculation for certain model problems whose exact eigenstates are known, Kan, et al. [7] have shown excellent agreement between the energies of these gauge invariant periodic solutions (for which we therefore suggest the name, "TDHF eigenstates") and the exact energy eigenvalues.

XVI. SUMMARY

The TDHF description of continuum reactions can be restructured from an initial-value problem into a form analogous to the S-matrix version of the Schrödinger theory. The resulting TD-$\mathscr{S}$-HF theory involves only self-consistent single determinantal solutions of the TDHF equations, and invokes time averaging to obtain a consistent interpretation of the TDHF analogs of quantities which are constant in the exact theory, such as the S-matrix and the asymptotic reaction channel properties.

Periodic TDHF solutions then play the role of stationary eigenstates in the construction of suitable asymptotic reaction channel states. If these periodic channel states occur only at discrete energies, then the resulting channels are mutually orthogonal (on the time average) and the theory exhibits a structure fully analogous to the exact theory.

In certain special cases where the periodic solutions are known to occur as an energy continuum, the requirement that the periodicity of the channel solutions be a gauge invariant property provides a natural requantization condition, which turns out to be identical with the Bohr-Sommerfeld quantization rule. Thus it emerges that the TD-$\mathcal{S}$-HF description can always exhibit a structure analogous to that of the Schrodinger reaction theory: the qualitative effect of the single determinantal assumption, overall, is to impose the requirement of time averaging upon the interpretation of the physical quantities in TD-$\mathcal{S}$-HF whose Schrödinger analogs are constant.

For nuclear structure physics, the "TDHF eigensolutions" offer a time-dependent description of stationary states which agrees well with the exact eigenstates for the model problems considered so far [7], and which invites comparison with the corresponding stationary RPA states.

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