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SINGLE DETERMINANTAL REACTION THEORY: ASYMPTOTICITY, PERIODICITY, TIME AVERAGING, CHANNEL ORTHOGONALITY, REQUANTIZATION AND GAUGE INVARIANCE

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SINGLE DETERMINANTAL REACTION THEORY: ASYMPTOTICITY, PERIODICITY, TIME AVERAGING, CHANNEL ORTHOGONALITY, REQUANTIZATION AND GAUGE INVARIANCE

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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 Schroedinger equation, the precise limits of its applicable physical range have remained largely unspecified. As a model of the Schroedinger system, deeper questions arise regarding the very physical interpretation of the TDHF solution for the reaction process: In what sense is it at all a proper Schroedinger 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?

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 propose that a consistent description of quantum reaction amplitudes, which is structurally fully analogous to the Schroedinger theory, can be built upon (the whole set of) self-consistent TDHF solutions, provided that the asymptotic channel states are built from gauge invariant periodic solutions, and the physical implications of the theory are interpreted on a time averaged basis.

II. COMMON VARIATIONAL ORIGINS OF TDHF AND SCHROEDINGER 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 non-relativistic time-dependent Schroedinger 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 Schroedinger 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-SCHROEDINGER PARALLELISM

The discussion will consider six interrelated aspects of the TDHF-Schroedinger 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 systems;

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 non-linear 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 problems to the same quantized states as the Bohr-Sommerfeld quantization rules would select).

IV. ASYMPTOTICITY IN A REACTION THEORY

In the exact Schroedinger 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 Schroedinger 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 Hartee-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-asympptoticity 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 systems, in pale contrast with the rich detail which the corresponding Schroedinger 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 such an interpretation would be found for the late time wave functions of conventional initial-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. TD-$\mathcal{S}$-HF: ASYMPTOTICITY AND PERIODICITY

In the TD-$\mathcal{S}$-HF restructuring of the single determinantal reaction theory [5], the S-matrix analog,

$$\mathcal{S}_{fi} = (T_2 - T_1)^{-1} \int_{T_1}^{T_2} <\Phi_f(\vec{x},t')|\Phi_i(\vec{x},t')>dt' \qquad (2)$$

describes the transition probability from an initial to a final self-consistent TDHF reaction channel. In reference [6] the form (2) for $\mathcal{S}$ is obtained heuristically by analogy with the exact Schroedinger 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 Schroedinger equation. In addition, the palpable physical error introduced by 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.

Under the ansatz (2) 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.

VII. 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 characteristics must be characterized by time averages (over the period) of physical operators. We note that also in the definition of $\bar{\mathscr{S}}$, the time average defined by equation (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 is to be obtained by time-averaging over the whole interaction interval.

VIII. 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

Schroedinger 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

$$a_{gf} = \langle \Phi_g(\vec{x},t) | \Phi_f(\vec{x},t) \rangle \qquad (3)$$

do not automatically vanish. It follows that under the statistical interpretation of quantum mechanical amplitudes, the statement that a system is described by the solution, Φ_f, must also assert with a probability, $|a_{gf}|^2$, 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 (3), but its time average value,

$$\overline{a_{gf}} = (2\tau)^{-1} \int_{t-\tau}^{t+\tau} \langle \Phi_g(\vec{x},t') | \Phi_f(\vec{x},t') \rangle dt' , \qquad (4)$$

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 $\{f\}$. (In equation (4), τ must be taken large enough for $\overline{a_{gf}}$ to be independent of the interval, τ; in the asymptotic region, this is always possible.) Then, as was shown in reference [6], the time averaged overlaps between distinct asymptotic channels,

$$\overline{a_{gf}} = 0, \qquad \{g\} \neq \{f\}, \qquad (5)$$

all vanish, 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 (5) 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.

IX. 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 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,

$$\Phi_p(\vec{x},t+T) = \Phi_p(\vec{x},t) \qquad (6)$$

or merely approximately so over some time interval.) Kan's work therefore forces one to deal with the Requantization process discussed in reference [5], 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 orthogonality, and therefore could not consistently predict physical measurements in one-to-one correpondence 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 reference [6].

We again proceed by analogy with the Schroedinger 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 continous, nevertheless the periodic solutions capable of playing the role of eigenstates, especially as regards gauge transformation properties, occur only as a discrete set.

X.GAUGE INVARIANCE OF THE TIME DEPENDENT SCHROEDINGER THEORY

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

$$\hat{H} = H + \beta(t) \tag{7}$$

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,

$$<\hat{\Psi}_i|\mathcal{O}(\vec{x},\vec{p})|\hat{\Psi}_j> \equiv <\Psi_i|\mathcal{O}(\vec{x},\vec{p})|\Psi_j>. \tag{8}$$

Equation (8) 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 reference [9].)

Note that among the physical observables, there must occur the energy operator, given by the Hamiltonian, $H(\vec{x},\vec{p})$. We have defined the gauge transformation (7) as a transformation of the time evolution operator only. Therefore the energy operator, like all the other operators for physical observables, is unaffected by it.

XI. GAUGE INVARIANCE OF EIGENSTATES

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

$$H\ \psi_\lambda(\vec{x}) = E_\lambda\ \psi_\lambda(\vec{x}). \tag{9}$$

(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 (7), of the form,

$$\Psi_\lambda(\vec{x},t) = \psi_\lambda(\vec{x})\ \exp - (i/\hbar)[E_\lambda(t-t_0) + \int_{t_0}^{t} \beta(t')dt'] \tag{10}$$

$$= \psi_\lambda(\vec{x})\ \exp - (i/\hbar) \int_{t_0}^{t} <\Psi_\lambda|\hat{H}(t')|\Psi_\lambda>dt'. \tag{11}$$

The latter form (11) is written to emphasize the fact that under gauge transformation, only the phase factor is altered, while the stationary state remains invariant. By analogy, then, we shall insist that the periodic channel solutions of TDHF must also be invariant under arbitrary gauge transformations.

XII. TD-$\mathscr{S}$-HF: PERIODIC STATES AS GAUGE ANALOGS OF EIGENSTATES

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

$$\mathscr{H}[\Phi]\cdot\Phi = \{\mathscr{H}^{o}[\Phi] + \langle\Phi|H - \mathscr{H}^{o}|\Phi\rangle\}\cdot\Phi = i\hbar\dot{\Phi} \tag{12}$$

and a specified initial-value determinant. The TDHF "Hamiltonian", $\mathscr{H}$, of equation (12) is uniquely prescribed [9] by the variational principle (1). Then $\mathscr{H}^{o}$ may be the conventional self-consistent Hartree-Fock Hamiltonian, or that Hamiltonian augmented by an arbitrary additive function of time only. Now consider the effect upon a periodic solution, $\Phi_p(\vec{x},t)$, of (12) of a gauge transformation (7). The new solution is related to the old by a phase factor,

$$\hat{\Phi}(\vec{x},t) = \Phi_p(\vec{x},t)\ \exp - (i/\hbar)\int_{t_0}^{t}\beta(t')dt'. \tag{13}$$

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 gauge 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.,

$$\Phi(\vec{x},t) = \Phi_p(\vec{x},t)\ \exp - (i/\hbar)\int_{t_0}^{t}\langle H(t')\rangle dt' \tag{14}$$

where Φ_p is a periodic function satisfying (6). A function of the form (14) will transform under the gauge transformation of H in precisely the same way as the exact solution (11), and the periodic solution, Φ_p, is precisely the analogy of the stationary eigenstate, $\psi_\lambda(x)$.

XIII. GAUGE INVARIANT TDHF EQUATION

Of course the function (14) must satisfy the TDHF equation (12) implied by the variational principle (1). Then the periodic factor, Φ_p, of (14) satisfies the following equation,

$$[\mathcal{H} - \langle\Phi_p|\mathcal{H}|\Phi_p\rangle]\Phi_p = i\hbar\dot{\Phi}_p. \tag{15}$$

We refer to (15) as the gauge invariant TDHF equation, since it is manifestly unaffected by any transformation of the form (7).

XIV. CONTINUATION OF PERIODIC TDHF SOLUTIONS: GAUGE REQUANTIZATION

For certain model problems, Kan shows that equation (12) 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 by the equality,

$$E = \langle\Phi_p|H|\Phi_p\rangle = 2N\pi\hbar/T \tag{16}$$

are of the form (14) with a periodic factor which satisifies the gauge invariant TDHF equation (15). Then (16) selects a discrete subset of the periodic continuum, for which the space-dependent periodic factor, Φ_p, is invariant under the gauge transformation (7), exactly as are the eigenstates of the exact Hamiltonian.

Thus, condition (16) offers a natural basis for the requantization of the continuum of periodic TDHF solutions. It selects those periodic states which remain periodic, just as the eigenstates remain stationary, under an arbitrary gauge transformation. In turn, the TD-$\mathcal{S}$-HF channel wave functions are all initializable in terms of specific periodic states, no matter what the choice of gauge. And their discreteness in energy guarantees also the mutual (time-averaged) orthogonality property (5) 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 (15) as acceptable channel states, rather than the continuous set of periodic solutions of (12). Finally, we note that Kan,et.al, [7] have also demonstrated the equivalence of the condition (16) with the Bohr-Sommerfeld quantization condition for the model examples they have analyzed, an intriguing coincidence which is still under study.

XV. 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 Schroedinger 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 labels.

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 (suggestively) turns out to be identical with the Bohr-Sommerfeld quantization rule.

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