PHYSICAL ASYMPTOTICITY IN NONLINEAR COLLISION THEORIES AND TIME AVERAGING OF GAUGE INVARIANT PERIODIC QUANTIZED SOLUTIONS[†]

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Introduction

In recent years several methods of utilizing nonlinear mean field propagation in time to describe nuclear reactions have been studied. They include the Initial Value Time-Dependent Hartree-Fock (TDHF) method,[1,2] the S-Matrix Time-Dependent Hartree-Fock (TD-S-HF) method,[3,4] and the Functional Integral Stationary Phase (FISP) method.[5-7] In each, one-body fields which are functionals of the time-dependent solutions are used to describe approximately the effects of the two-body interactions of the exact system.

We here address the question when such theories have the qualitative property of physical asymptoticity (discussed more precisely below), without which their predictions can, as of matter of principle, be of little practical value. We show that physical asymptoticity can be assured only when the approximate S-matrix amplitudes are constant, and for nonlinear theories also only by a proper a priori choice of the asymptotic reaction channel states. Such a choice therefore becomes an essential element of the reaction theory itself.

In the single-determinantal TDHF case the need to select channel states leads to the question of which single-determinantal bound state solutions are the proper analogs of exact eigensolutions, an answer to which was provided by the Gauge Invariant Periodic Quantization (GIPQ) method.[8-10] But when the generalized GIPQ method is applied in the full space of the Schrödinger equation, it yields not just all of the exact eigenstates, but an infinity of additional, physically spurious states. Thus arises a fundamental many-to-one ambiguity in the correspondence between GIPQ solutions and exact eigensolutions.

Some results of a recent study[11] of time averaging as an interpretative procedure for extracting the physical content of the bound state GIPQ solutions are reported here. In the full Schrodinger space, direct time averaging annihilates every physically spurious GIPQ solution, and projects each of the others onto the corresponding exact eigensolution. Thus, time averaging emerges from this test as a plausible general criterion for rejecting physically spurious GIPQ solutions. If it suffices for that role, then it could provide a correspondence (e.g.) between the exact eigenstates and the physical GIPQ solutions.

As an incidental by-product, the present analysis suggests a new, properly asymptotic, Hartree-Fock Stationary Phase S-matrix amplitude[12] which utilizes the FISP method only within the collision interval; outside of the collision interval

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properly selected asymptotic channel solutions propagate by the Dirac-TDHF dynamics.[13] This new amplitude therefore joins that of the TD-S-HF theory as the second S-matrix approximant to be obtained from a physically asymptotic nonlinear theory.

Physical Asymptoticity

Physical Asymptoticity is that property of a reaction theory which guarantees that its predictions for the internal properties of the emergent reactants will be independent of the precise (distant) location of the measuring apparatus. As we shall illustrate in the case of the Schrödinger theory, this property follows from the constancy of the S-matrix expansion coefficients ("coefficient asymptoticity") and from the existence of channel states in which packets translate through space without alteration of the internal properties of the fragment ("channel asymptoticity"). The latter property stems essentially from the translational invariance of the interactions in the Hamiltonian, which implies the complete dynamical separation of the motion of its center of mass from the internal motions of a composite fragment. Thus once such a fragment is isolated, its center of mass translation and its internal dynamical evolution proceed separately and independently. Hence the familiar freedom always to choose the overall "center of mass" coordinate system without loss of generality, but also the result for "scattering systems" that the internal motion of each isolated fragment will evolve without coupling to the uniform translational motion of its center of mass.

"Scattering systems" are those[14] for which the interactions are of sufficiently short range that the complete Hamiltonian reduces at large fragment separations to the sum of isolated Hamiltonians, one for each fragment; i.e., for which

$$H = H_c^0 + V_c \xrightarrow[|\vec{R}_{12}| \to \infty]{} H_c^0 = H_{c,1}^0 + H_{c,2}^0 \qquad (1)$$

where $H_{c,i}^0$ is the sum of the center of mass (kinetic energy) Hamiltonian of fragment i in channel c and the internal Hamiltonian of that fragment, and $\vec{R}_{12}$ is the fragment separation. Since our discussion is not concerned with the nuances of marginally short range forces, we assume that V_c is zero outside of some finite range, so that for each channel the fragment separation space is divided sharply into an external region and a collision volume. Correspondingly, for our localized packets,† the time is separated into the early and late asymptotic intervals and a collision interval.

For such systems, the independence of the center of mass and internal motions applies not just to the system as a whole, but also to individual channel fragments

†Throughout this paper we discuss the time-dependent scattering theory, and assume that the center of mass motions of the composite reactants are described by localized packets.

in the external region where the condition (1) prevails. Thus (1) guarantees that each channel wave function can be written in the external region as a product of packets describing the motions of the centers of mass and internal wave functions for each of the products.

Physical Asymptoticity in the Exact Schrödinger Theory

In the time-dependent Schrödinger description of a scattering system, an S-matrix amplitude is given by the overlap,

$$S_{fi} = \langle \Psi_f^{(-)}(\vec{x},t) | \Psi_i^{(+)}(\vec{x},t) \rangle \tag{2}$$

between one exact solution, $\Psi_i^{(+)}$, initialized early as well-separated approaching packets, $\Phi_i(\vec{x},t)$, and another, $\Psi_f^{(-)}$, initialized late as emerging packets, $\Phi_f(\vec{x},t)$. Thus

$$\lim_{t \to \mp \infty} \Psi_c^{(\pm)}(\vec{x},t) \to \Phi_c(\vec{x},t). \tag{3}$$

The channel labels c must suffice to initialize a unique solution of the time-dependent Schrödinger equation, including the internal wave function of each fragment and the motion of its center of mass. Since S_{fi} in (2) is constant in time (by the Schrödinger equation itself), the coefficients in

$$\Psi_i^{(+)}(\vec{x},t) = \sum_f S_{fi} \Psi_f^{(-)}(\vec{x},t) \tag{4}$$

$$\xrightarrow[t \to +\infty]{} \sum S_{fi} \Phi_f(\vec{x},t) \tag{5}$$

are constant in time.

If the channel label f includes the specification of a set of eigenvalues, say $\{m_f\}$, of an exhaustive set of internal operators $\{M\}$, then the probability of measuring such a set is simply $P_{\{m_f\}} = |S_{fi}|^2$ and remains constant as the packets of Φ_f propagate outward in time.

But if instead of f, one had initially chosen some other set of channel labels, say g, which did not include an exhaustive set of internal eigenvalues (or perhaps not the particular exhaustive set of eigenvalues desired), then a time-independent unitary transformation, A, among the internal channel states will form the desired channel states, f, from the states, g, so that the new basis, obtained by the replacement,

$$X_g(\vec{x},t) = \sum_f A_{fg} \Phi_f(\vec{x},t), \tag{6}$$

is labelled directly by the measurables $\{m_f\}$ of f. Because of the linearity of H, the Φ_f are surely Schrödinger solutions if only the X_g were solutions. Because of the constancy of the unitary transformation U_{fg}, which depends upon the guaranteed asymptotic separation of the internal and translational motion, the final probability of measuring the eigenvalues $\{m_f\}$ is still constant in time,

$$P_{\{m_f\}} = |\sum_g A_{fg} S_{gi}|^2 \tag{7}$$

so that the probability of measuring the set $\{m_f\}$ is independent of time and therefore of the location of the measuring apparatus. Thus it follows that the Schrödinger system is physically asymptotic.

Asymptoticity is Ubiquitous in Schrödinger Theory

We note that the physical asymptoticity of the Schrödinger scattering systems requires (a) constant S matrix, (b) the asymptotic separation of the translational and internal motions of the separate fragments, and either (c) an a priori choice of channel states labelled by the eigenvalues of the desired exhaustive set of measurements or (d) a unitary transformation relabelling the channels by such a set.

But "coefficient asymptoticity", (a), is guaranteed by the definition (2) of the S matrix and the time-dependent Schrödinger equation. And "channel asymptoticity" is implied by properties (b) and (d), of which (b) follows from the translational invariance of the interactions and the asymptotic condition (1) for scattering systems, and (d) is always an available option, by virtue of the linearity of the theory. Thus physical asymptoticity is automatically a property of the Schrödinger collision theory of scattering systems. This may partially explain why it is sometimes either taken erroneously for granted or overlooked in the study of alternative collisions theories.

Nonlinear Approximate Theories May Not Be Physically Asymptotic

In contrast with the Schrödinger theory, approximate theories are likely to lack one or more of these conditions for physical asymptoticity unless explicitly constructed to include them. In particular since nonlinearity voids the superposition principle, option (d) above is not available in mean field theories. This implies that properly asymptotic channels, if they exist at all, must be selected a priori, and used exclusively to describe all motions in the asymptotic regions (1). Otherwise channel asymptoticity will be lacking. But independently, coefficient asymptoticity may fail if in the approximate analog of the expansion (5), the coefficients, comprising the approximate S-matrix elements of the theory, are not constant in time. We emphasize that physical asymptoticity, which speaks to measurements in the asymptotic region, requires both coefficient asymptoticity and channel asymptoticity.

Because TDHF Translations Separate from Internal Motions, Channel Asymptotic TDHF Solutions Exist

In the Dirac-TDHF dynamics a set of channel asymptotic states always exists, due to a remarkable parallel between the TDHF system and the Schrödinger system, as follows: under TDHF time evolution, the expectation value of every one-body operator which commutes with the exact Hamiltonian remains constant.[15] Since the total momen-

tum, $\vec{P}$, is such a one-body operator, its expectation value remains constant under TDHF evolution. The result is that a whole continuum of TDHF solutions initialized at t_i by the functions,

$$\Phi_{\vec{K}}(\vec{x},t_i) = \Phi_0(\vec{x},t_i) \exp i \vec{K}\cdot\vec{R} \tag{8}$$

(where $\vec{R} = A^{-1}\sum \vec{x}_i$ is the center of mass coordinate and $\vec{x}$ denotes the whole set of A coordinates, $\vec{x}_i$), and parametrized continuously by the mean total momentum vector, $\vec{K}$, correspond to precisely the same time-dependent internal state. For if $\Phi_0(\vec{x},t)$ is a zero-momentum time-dependent constant-<H> Hartree-Fock solution,[16] then

$$\Phi_{\vec{K}}(\vec{x},t) = \Phi_0(\vec{x}_i - \hbar\vec{K}t/AM,t) \exp i (\vec{K}\cdot\vec{R} - \hbar^2 K^2 t/2AM) \tag{9}$$

is another TDHF solution whose internal evolution in the fragment's average center of mass frame is identical with that of Φ_0 in the laboratory frame.

Thus it follows that from each TDHF solution whose measurable internal physical properties remain constant in time, translating solutions whose measurable internal properties are guaranteed to remain constant in time may be constructed by (9). In this way, each stationary Hartree-Fock solution becomes a prospective channel asymptotic state for a physically asymptotic TDHF collision theory. And if periodic states are interpreted in terms of the progressive phase averages, discussed below, over these periods,[4,11] they, too, may serve as channel asymptotic states when made to translate as in (9) above.[17]

Initial Value TDHF Theory is Non-Asymptotic

Nevertheless, the Initial Value TDHF reaction theory, which has in recent years been the object of the extensive numerical computation,[2] is decidedly not a physically asymptotic theory. Initial Value TDHF assumes an initial state in which two well-separated Hartree-Fock ground states translate towards one another, and utilizes the Dirac-TDHF time evolution to carry the system into and through the collision and the re-separation of the density into spatially disconnected parts, which then translate apart.

Although the assumed initial state happens to be an acceptably asymptotic channel, so that its early time behavior incorporates correct channel asymptoticity, Initial Value TDHF does not lead to physically asymptotic late time solutions because the expansion, analogous to (5) above of its late-time solution onto any set of channel asymptotic states will in general exhibit coefficients with nontrivial time dependence, and have been found to do so in the many numerical calculations discussed in Ref. 2. Therefore, its predictions for the results of internal physical measurements change* as the wave packet propagates outward in time. Thus the predictions of initial value TDHF for physical measurements on the emergent fragments depend upon the precise location of the measuring apparatus, even when it is in the asymptotic region well outside the collision volume.

* excepting those[15] which correspond to one-body operators which commute with H.

TD-S-HF Theory is Asymptotic By Construction

Like Initial Value TDHF theory,[1,2] the TD-S-HF theory[3,4] also assumes that all time evolution proceeds according to the Dirac-TDHF equation.[13] But it builds the theory entirely upon solutions which, either at early or at late times, reduce to the channel asymptotic TDHF solutions discussed above. Since the overlap of such solutions (analogous to Eqs. (2) for S) is not time independent, TD-S-HF utilizes a time average over the collision interval to define constant coefficients for the expansion analogous to (5). It therefore achieves channel asymptoticity by the explicit choice of the solutions allowed, and coefficient asymptoticity by using time averaging to extract a constant S-matrix analog.

Although this procedure is intuitive and heuristic, it results in a proper physically asymptotic theory whose predictions for measurements of the internal properties of the emergent fragments, unlike those of physically non-asymptotic theories, are stable over the range of space and time outside the collision volume. One might also mention that it has also been constructed so as to reduce precisely to the correct exact theory whenever the system is exactly described by the Dirac-TDHF theory.

Functional Integral Stationary Phase Mean Field Theories Are Not Asymptotic

The FISP theory of many-body collisions is constructed by approximating the exact Schrödinger expression for the time-propagator by a stationary phase approximation to a functional integral.[5] It leads to a coupled pair of first-order time-dependent equations which somewhat resemble Dirac-TDHF equations, and opens a whole range of interesting questions and possibilities in the many-body reaction theory.

As regards asymptoticity, however, there seems no reason to believe that FISP theory is either channel asymptotic or coefficient asymptotic. In a later application,[6] the possibility of coefficient asymptoticity was kept open by utilizing a kind of approximate interaction representation, in which the calculated S matrix becomes independent of the asymptotic initial and final time limits of the calculation by virtue of the mutual cancellation of the time dependences of two approximate factors. However, this particular restructuring omits any consideration of channel asymptoticity and is therefore insufficient to assure physical asymptoticity.

Indeed, even if a selection criterion upon the initial and final states allowed in the FISP S-matrix theory were adopted, under which they were required to be channel asymptotic single determinants of the form (9), it seems unlikely that the FISP time evolution equations can allow them to remain so, since it offers no apparent mechanism for keeping the internal and translational motions uncoupled during the propagation outside the collision interval. On the other hand, the FISP approximation to the dynamics can be incorporated into a new, physically asymptotic description by reverting to Dirac-TDHF propagation in the asymptotic region, as we now discuss.

A Physically Asymptotic Hartree-Fock Stationary Phase (AHFSP) Theory

Just as the TD-S-HF theory was structured explicitly to provide physical asymptoticity together with Dirac-TDHF propagation in time, one can also construct a physically asymptotic theory in which the Functional Integral Stationary Phase approach provides the description of the dynamical evolution during the collision.[12] In this approach, the FISP method is utilized to define the amplitude that a state, $\Phi_i(\vec{x},T_1)$, at the beginning of the collision interval propagates into a state $\Phi_f(\vec{x},T_2)$ at the end of the collision interval, thereby defining a definite constant S-matrix approximent, and guaranteeing coefficient asymptoticity for the theory. Then channel asymptoticity is guaranteed by utilizing exclusively the channel asymptotic TDHF solutions discussed above, propagated by the Dirac-TDHF equation, outside of the collision interval.

The resulting Asymptotic Hartree-Fock Stationary Phase S-matrix element is given by the expression

$$S_{fi}^{AHFSP} = \langle \Phi_f^{(-)}(\vec{x},T_2) | U_{fi}^{FISP}(T_2,T_1) | \Phi_i^{(+)}(\vec{x},T_1) \rangle \qquad (10)$$

and provides the coefficient of the channel asymptotic TDHF solution, $\Phi_f^{(-)}(\vec{x},t)$, in the expansion analogous to (5). Here $U_{fi}^{FISP}(T_2,T_1)$ symbolizes the Functional Integral Stationary Phase approximate transition amplitude[5] from Φ_i at T_1 to Φ_f at T_2.

It is noteworthy that the amplitude S_{fi}^{AHFSP} is determined entirely by the dynamical behavior within the collision interval, (T_1,T_2). This feature is agreeably commensurable with the fact that in the exact theory all of the essential physical behavior is determined during the collision interval while only trivial translation and unperturbed time evolution occurs outside that interval.

The determination of the S matrix entirely within the collision interval is a feature that S_{fi}^{AHFSP} shares with the corresponding TD-S-HF amplitude, given by the expression,

$$S_{fi}^{TDSHF} = (T_2-T_1)^{-1} \int_{T_1}^{T_2} dt' \langle \Phi_f^{(-)}(\vec{x},T_2) | U_f^{TDHF}(T_2,t')^{\dagger} \, U_i^{TDHF}(t',T_1) | \Phi_i^{(+)}(\vec{x},T_1) \rangle . \qquad (11)$$

Here, e.g., the symbol, $U_i^{TDHF}(t',T_1)$, represents the Dirac-TDHF propagation of $\Phi_i^{(+)}(\vec{x},t)$ from time T_1 to time t'.

It is especially interesting to inquire about possible relationships between these two expressions, which constitute the only examples so far of S-matrix approximants from physically asymptotic nonlinear theories.

Time Averaged Periodic Solutions as Stationary Solutions

Early in the study of mean field reaction theories, the possibility of building asymptotic channel states on periodic TDHF solutions was advanced.[3] It was physically motivated by the fact that properly time averaged properties of such solutions

might serve as the TDHF analogs of stationary exact eigenvalues, allowing thereby approximate periodic states to serve the role of exact stationary eigenstates.

Subsequently, it was realized that the casting of periodicity as a physically essential property implied that it ought to be gauge invariant, like all the other physical properties of the nonrelativistic theory. This condition lead to a discrete quantization of the periodic solutions, and to the Gauge Invariant Periodic Quantization (GIPQ) method.[8-10] Later it emerged that the FISP approximation to the poles of $(E-H)^{-1}$ yields precisely the same spectrum as the (GIPQ) method.[18,19] We turn now to a brief summary of some recent developments[11] in the GIPQ method.

Gauge Invariant Periodic Quantization of Exact Schrödinger Solutions

The Gauge Invariant Periodic Quantization procedure seeks time-dependent GIPQ solutions of the form

$$\Phi(\vec{x},t) = \Phi_{GP}(\vec{x},t) \exp(-i\langle H\rangle t/\hbar). \tag{11}$$

where Φ_{GP} is the time-periodic analog of an exact gauge invariant stationary eigensolution.[8-10] The method may be applied to the TDHF single-determinantal subspace, or to any time-dependent parametric subspace of the full space.[10] In particular, Φ may be defined in the full space of the exact Schrödinger eigensolutions. In that case, one would expect the set GIPQ solutions to reduce to the set of exact eigensolutions.

For an exact Schrödinger solution, of the form

$$\Psi(\vec{x},t) = \sum_n a_n \psi_n(x) \exp(-i E_n t/\hbar) \tag{12}$$

the Gauge Invariant Periodic Quantization condition requires the form (11):

$$\Psi(\vec{x},t) = \{\sum_n a_n \psi_n(x) \exp(-it[E_n-E])\}\{\exp(-iEt/\hbar)\} \tag{13}$$

where the first factor is periodic and where $\langle H\rangle = E = \sum_n |a_n|^2 E_n$. Periodicity requires that the frequency of every term must be an integral multiple, say k_n, of some fundamental frequency, Ω, so that

$$(E_n-E) = \hbar k_n \Omega \qquad (k_n \text{ an integer}) \tag{14}$$

for every n value for which $a_n \neq 0$.

Spurious GIPQ States Occur But Are Deleted by Progressive Phase Averaging

The exact eigensolutions $E = E_n$, $a_n = 1$, are evidently always included among the GIPQ solutions honoring (13). But in addition, an infinity of two-component solutions exists which are not exact eigensolutions, and which therefore are to be considered physically spurious. They pose the question how one is to select the physical GIPQ solutions from the spurious ones.

From the same physical viewpoint as that which suggested periodic functions in the first place [3,17] (namely, that under a time averaged interpretation periodic functions can describe constant physical characteristics), one naturally inquires about time averaging, and finds immediately that the time average of the Gauge Invariant factor in (13) is given by [11]

$$\overline{\psi_{GP}(\vec{x},t)} = \lim_{\tau\to\infty} (2\tau)^{-1} \int_{t-\tau}^{t+\tau} dt' \sum a_n \psi_n(x) \exp(-it'[E_n - E]/\hbar) \tag{15a}$$

$$= \sum_n a_n \psi_n(x)\ \delta(E_n - E), \tag{15b}$$

equal to zero unless the energy equals one of the eigenergies, and equal to $a_n\psi_n(x)$ when $E = E_n$. Thus time averaging in the full space annihilates all the spurious GIPQ solutions, and projects the (unnormalized) exact spatial eigenfunctions from the non-spurious ones, providing thereby a valid criterion for selecting the physical GIPQ solutions out of the set of all GIPQ solutions.

This exercise in the full eigenfunction space therefore provides no deterrent to the prospect that in more restricted approximate subspaces, time averaging might also serve to eliminate spurious solutions and to provide a correspondence between the physical GIPQ solutions and the (perhaps only approximate) eigensolutions obtained by other methods (such as, e.g., stationary state diagonalization via RPA, Tamm-Dancoff, etc.).

It should be noted that for periodic solutions time averaging is equivalent to averaging over a real-valued "progressive phase" parameter which increases monotonically by 2π during each period. Indeed, this view of the averaging as a "progressive phase" rather than a time averaging is distinctly preferable when one addresses the collision problem, since the translating periodic solutions depend upon time both because of the genuine physical translation in space and time and because of the periodic internal oscillation of the solution, which is viewed as non-physical behavior to be removed by the averaging. Then the progressive phase prescription of the average neatly selects and properly executes only the average only over the periodic variation.

Summary

The property of physical asymptoticity, which guarantees that a reaction theory's predictions for physical measurements of internal fragment properties shall not depend upon the precise location of the measuring apparatus, has here been analyzed in some detail. Since the lack of such a property reduces most of the nontrivial physical content of an approximate many-body reaction theory to practical unobservability, this property warrants some attention.

We find that physical asymptoticity is guaranteed in the Schrödinger collision theory of scattering systems with translationally invariant interactions by the constancy of the S-matrix elements (which we label "coefficient asymptoticity") and by the decoupling of the internal and translational motions for well-separated fragments ("channel asymptoticity"). Both conditions are necessary for physical asymptoticity.

For nonlinear approximants to the Schrödinger theory, a specific a priori selection of asymptotic channel states seems necessary to achieve channel asymptoticity. Within the Dirac-TDHF dynamics such a set does exist, so that channel asymptotic single-determinantal propagation can be described by Dirac-TDHF time evolution. But it is not clear that such a set exists for the propagation of well-separated fragments under the FISP approximate time evolution.

A review of nonlinear mean field many-body reaction theories shows that Initial Value TDHF (by far the most computed theory) is non-asymptotic, as is the FISP theory (even in the coefficient asymptotic form of Alhassid and Koonin,[6] since that description is still channel non-asymptotic). The TD-S-HF theory is asymptotic by construction

A new Asymptotic Hartree-Fock Stationary Phase (AHFSP) description[12] which utilizes Dirac-TDHF channel solutions and propagation outside the collision interval, and the FISP method to describe the dynamical evolution within the collision interval, is reported. Together with the TD-S-HF theory it constitutes the second example of a physically asymptotic nonlinear many-body reaction theory. Although the S-matrix approximants of these theories are evidently different, their careful comparison should prove enlightening.

The Gauge Invariant Periodic Quantized solutions of the exact Schrödinger problem are considered to test whether they include as they ought the exact eigenfunctions. They do, but include as well an infinity of spurious solutions. However, time averaging over the periodic motions (or better stated, "progressive phase averaging") annihilates all the spurious solutions, and projects the physical solutions onto the exact (but unnormalized) eigensolutions. These results offer no discouragement for the prospect that in more restrictive approximate subspaces progressive phase averaging of GIPQ solutions may reject physically spurious solutions and provide a correspondence between the remaining solutions and the (exact or approximate) eigensolutions obtained by stationary state methods.[11]

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