Physical interpretation and quantization of periodic time-dependent Hartree-Fock solutions

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We outline several sets of physical conditions which lead to periodic or multiply periodic solutions of the time-dependent Hartree-Fock equations. In every instance the Fourier components can be identified with transition matrix elements of the density fluctuation operator between collective eigenstates of the system. A simple variational derivation of the Bohr-Sommerfeld quantization condition for such solutions is described.

I. INTRODUCTION

A few years ago there was considerable interest in the theory and quantization of periodic solutions of the time-dependent Hartree-Fock (TDHF) equations.[1-4] Currently there is intense interest in constructing and utilizing such solutions.[5-7] In this report we shall revisit the earlier scene, partly with the intention of tying it in with the current one.

One aim of the current work is to present a "new" derivation of the quantization condition which we consider simpler and more direct than those appearing in the literature. Though admittedly the definition of simple has some relation to taste and previous experience, it is undeniable that the previous work does not provide a clear physical interpretation of the periodic density matrix, which is the prime physical object computed by the theory.

It is, of course, easy to guess[5-7] the required interpretation: The Fourier components of the density matrix are transition matrix elements between discrete states of the system, states assembled into a collective band. This interpretation is suggested by the notions of matrix mechanics and the ideas that led to its conception[8] through the aid of the correspondence principle. In the past, one of us has shown how these ideas could be refined and applied to the derivation of the WKB approximation, both in particle quantum mechanics[9,10] and for simple quantum field theories containing soliton solutions.[11] The purpose of this relatively brief report is to translate the methods of Ref. 11 into the nuclear physics domain, thereby "filling a gap in the literature."

These methods are based on the following ideas (which have far from outlived their usefulness): It is a truism that any solution of HF or TDHF theory somehow describes the properties of a wave packet of eigenstates. If this is so, then a clear *modus operandi* presents itself. Starting with Heisenberg's equation of motion for a density operator and forming suitable matrix elements, we may look for operations and approximations by which we can derive, i.e, justify, the TDHF limit. The bewildering flexibility of physical applications (large amplitude collective motion, periodic motion, and heavy-ion scattering to mention the most prominent of the currently interesting ones)

suggests that the derivation must in part be tailored to the individual physics problem. This is because we must discover which packet of quantum mechanical amplitudes is relevant to the given case. At the same time there must be a general pattern which guarantees the Slater determinantal character of the final result. This pattern we believe to be a generalized factorization approximation for the two-particle density matrix elements, which has the proper classical limit.[12] This limit can be achieved provided the quantity which is to satisfy TDHF theory is a suitable Fourier (series or integral) superposition of quantum amplitudes. In the present example we deal with a Fourier series with a fundamental frequency which is approximately an energy difference (for the simply periodic case).

The detailed derivation of TDHF for periodic solutions is given in Sec. II, where we believe we have managed to mention all cases of possible physical interest. The intuitively appealing interpretation of the Fourier coefficients is established. In Sec. III we provide two simple alternatives for the quantization condition. The first, based directly on the correspondence principle, requires no derivation to speak of but may be of limited use in the many-body problem. The second, favored in the nuclear physics literature,[1-4] is derived in a few lines from a quantum-classical version of the principle of least action.[9-11]

The interesting problem remaining at this point is the development of efficient methods for the generation of periodic or quasiperiodic solutions of the resulting nonlinear equations.

II. PHYSICAL INTERPRETATION OF PERIODIC SOLUTIONS OF TDHF

A. Classical limit

We study a standard nonrelativistic nuclear Hamiltonian ($\hbar = m = 1$),

$$H = \int dx \, \psi^\dagger(x)(-\tfrac{1}{2}\nabla^2)\psi(x)$$
$$+ \tfrac{1}{4} \int dx_1 \cdots dx_4 \psi^\dagger(x_1)\psi^\dagger(x_2)$$
$$\times V(x_1 x_2 \mid x_3 x_4)\psi(x_4)\psi(x_3) . \qquad (2.1)$$

Here, $\psi(x)$ and $\psi^\dagger(x)$ are single nucleon destruction and creation operators, V is an antisymmetric matrix element of the interaction, and x refers to all single particle degrees of freedom. We shall repress any explicit reference to spin and charge in the following.

In this section our aim is to provide a physical interpretation of periodic solutions of TDHF. We shall carry out the argument for simply periodic functions, but it can be extended without difficulty to multiply periodic behavior. The argument has two parts. (i) We define a superposition of matrix elements of the density operator which in the correspondence principle limit takes the form of a Fourier series in time (a periodic function). (ii) We examine the Heisenberg equations of motion for such matrix elements and look for conditions under which TDHF can be derived. We apply a generalized factorization of two-particle density matrices[12] and then take the correspondence limit of the equations of motion. The same sequence of arguments leads to the condition "$\rho^2=\rho$" which characterizes determinantal solutions.

We thus assume that the many-body Hilbert space supports an approximately decoupled one-dimensional space of collective states $|n\rangle$ specified by an integer n, where $|0\rangle$ is the ground state. Let E_n be the energy of state $|n\rangle$. The matrix element

$$\rho(x_1 tn \mid x_2 tn') \equiv \langle n' \mid \psi^\dagger(x_2 t)\psi(x_1 t) \mid n \rangle$$
$$= \exp[i(E_{n'}-E_n)t]\langle n' \mid \psi^\dagger(x_2)\psi(x_1) \mid n \rangle \tag{2.2}$$

can be written in the approximate form

$$\rho(x_1 tn \mid x_2 tn') \cong \rho_{\bar{n},\nu}(x_1 x_2)e^{iw(\bar{n})\nu t}, \tag{2.3}$$

i.e., as the νth term in a Fourier series provided we define

$$n'=\bar{n}+\tfrac{1}{2}\nu, \quad n=\bar{n}-\tfrac{1}{2}\nu, \tag{2.4}$$

and set

$$E_n-E_{n'} \cong \left[\frac{dE_{\bar{n}}}{d\bar{n}}\right]\nu=w(\bar{n})\nu, \tag{2.5}$$

and provided the matrix elements $\rho_{\bar{n},\nu}$ are sensibly different from zero only as long as $\nu \ll \bar{n}$: This is the correspondence principle limit which (in general) requires that $\rho_{\bar{n},\nu}$ be a slowly varying function of $\bar{n}$ and a rapidly decreasing function of $|\nu|$. Under these conditions,

$$\rho_{\bar{n}}(x_1 x_2 \mid t)= \sum_\nu \rho(x_1 tn \mid x_2 tn') \tag{2.6}$$

is a periodic function of t with period $T_n=2\pi/w(\bar{n})$.

Next, consider the Heisenberg equation of motion,

$$i\partial_t\psi^\dagger(x_2 t)\psi(x_1 t)= -\tfrac{1}{2}(\nabla_1^2-\nabla_2^2)\psi^\dagger(x_2 t)\psi(x_1 t)+\tfrac{1}{2}\int \psi^\dagger(x_2)\psi^\dagger(x_3)V(x_1 x_3 \mid x_4 x_5)\psi(x_5)\psi(x_4)$$
$$-\tfrac{1}{2}\int \psi^\dagger(x_3)\psi^\dagger(x_4)V(x_3 x_4 \mid x_2 x_5)\psi(x_5)\psi(x_1), \tag{2.7}$$

and form the average defined in (2.6). Let us study, for example, the first of the interaction terms in (2.7). We have

$$\sum_\nu \langle n' \mid \psi^\dagger(x_2 t)\psi^\dagger(x_3 t)\psi(x_5 t)\psi(x_4 t) \mid n \rangle \cong \sum_\nu e^{iw(\bar{n})\nu t} \sum_{n''} \tfrac{1}{2}\{\langle n' \mid \psi^\dagger(x_2)\psi(x_4) \mid n''\rangle\langle n'' \mid \psi^\dagger(x_3)\psi(x_5) \mid n \rangle$$
$$-(2\leftrightarrow3)-(4\leftrightarrow5)+(2\leftrightarrow3, 4\leftrightarrow5)\}, \tag{2.8}$$

which involves the application of the correspondence principle in the exponent and the application of the generalized Hartree-Fock factorization of the two-body density matrix alluded to above. We wish to reduce the right hand side of (2.8) to the usual antisymmetric product, characteristic of Hartree-Fock theory. Notice that with the definition

$$\nu'=n-n', \tag{2.9}$$

we have, e.g.,

$$\sum_{n''} \langle n' \mid \rho \mid n''\rangle\langle n'' \mid \rho \mid n \rangle = \sum \rho_{\bar{n}', \nu-\nu'}\rho_{\bar{n}'',\nu} \cong \sum \rho_{\bar{n}, \nu-\nu'}\rho_{\bar{n},\nu}. \tag{2.10}$$

Here we have defined $\bar{n}'=\tfrac{1}{2}(n'+n'')$, $\bar{n}''=\tfrac{1}{2}(n+n'')$, and then invoked the assumption of slowly varying behavior in $\bar{n}$. By writing $\nu=\nu-\nu'+\nu'$ in the exponent in (2.8), Eq. (2.10) easily yields the result

$$\rho_{\bar{n}}(x_4 x_5, x_3 x_2 \mid t) \equiv \sum_\nu \langle n' \mid \psi^\dagger(x_2 t)\psi^\dagger(x_3 t)\psi(x_5 t)\psi(x_4 t) \mid n \rangle \cong \rho_{\bar{n}}(x_4 x_2 \mid t)\rho_{\bar{n}}(x_5 x_3 \mid t)-\rho_{\bar{n}}(x_5 x_2 \mid t)\rho_{\bar{n}}(x_4 x_3 \mid t). \tag{2.11}$$

Finally, by applying (2.11) to the equation of motion (2.7), we find the TDHF equation

$$i\dot\rho_{\bar{n}}(x_1 x_2 \mid t)=[\mathcal{H}_{\bar{n}},\rho_{\bar{n}}](x_1 x_2 \mid t), \tag{2.12}$$

where

$$\mathcal{H}_{\bar{n}}(x_1 x_2 \mid t)=h(x_1 x_2)+V_{\bar{n}}(x_1 x_2 \mid t), \tag{2.13}$$

$$V_{\bar{n}}(x_1 x_2 \mid t)= \int V(x_1 x_3 \mid x_2 x_4)\rho_{\bar{n}}(x_4 x_3 \mid t), \tag{2.14}$$

and $h(x_1 x_2)$ is the single particle part of the nuclear Hamiltonian, represented as the kinetic energy operator in (2.1).

In addition to (2.12)–(2.14), it can be verified from (2.6) that

$$\int \rho_{\bar{n}}(xx \mid t)=N, \tag{2.15}$$

where N is the number of nucleons. From (2.11) and

(2.15), a standard derivation [set $x_3 = x_5$ and integrate, using (2.15)] yields

$$\int dx\, \rho_{\bar{n}}(x_1 x \mid t) \rho_{\bar{n}}(x x_2 \mid t) = \rho_{\bar{n}}(x_1 x_2 \mid t) . \qquad (2.16)$$

In summary, we have found that periodic solutions of TDHF can be interpreted as Fourier series with coefficients which constitute an array of transition matrix elements of the density matrix. This result is the field analogue of one that goes back to the origin of quantum mechanics.[8]

B. RPA limit: Nearly harmonic spectrum

The random phase approximation (RPA) limit can be derived in two ways using the methods of subsection A. First, we proceed, as is most conventional,[13] directly from the TDHF equation. Assume that in the neighborhood of a given average n, the diagonal element $\rho_{\bar{n},0}$ is dominant (of zero order), that the off-diagonal elements $\rho_{n,\pm 1}$ are first order, and that all other elements can be ignored. If $\rho_{n,0}$ is identified with the ground state Hartee-Fock density matrix, these assumptions yield, as is well known, static Hartree-Fock plus RPA equations.

A second fully quantum mechanical derivation also has considerable lineage.[14] In this derivation we may proceed as in (2.7) and (2.8), but we restrict n and n' to the values 0 or 1, and also restrict the selection rule for transitions induced by a density operator to $\Delta n = 0, \pm 1$. One further approximation (no-blocking approximation), namely

$$\langle 1 \mid \rho \mid 1 \rangle \cong \langle 0 \mid \rho \mid 0 \rangle , \qquad (2.17)$$

allows us to derive a linearized version of TDHF for a periodic density matrix $\rho(x_1 x_2 \mid t)$ which has the form

$$\begin{aligned} \rho(x_1 x_2 \mid t) = &\langle 0 \mid \psi^\dagger(x_2)\psi(x_1) \mid 0 \rangle \\ &+ \langle 1 \mid \psi^\dagger(x_2)\psi(x_1) \mid 0 \rangle e^{iwt} \\ &+ \langle 0 \mid \psi^\dagger(x_2)\psi(x_1) \mid 1 \rangle e^{-iwt} , \end{aligned} \qquad (2.18)$$

where $w = E_1 - E_0$. This form of the derivation is thus fully quantum mechanical in the sense that w is an energy difference and not a correspondence principle frequency that has to be reinterpreted.

This last remark suggests one more possibility. If the collective spectrum is nearly harmonic, at the same time that higher harmonics of the transition density, though decreasing with v, are nevertheless nonvanishing, then the TDHF equation for periodic solutions [Eq. (2.12)] can be derived without recourse to the approximation (2.5). The frequency w is then independent of $\bar{n}$ and equal to the first excitation energy. This possibility is realized for the low-lying monopole spectrum built on the isomeric state of ^{24}Mg.[6,7]

III. QUANTIZATION OF PERIODIC SOLUTIONS

In this section we shall discuss semiclassical (Bohr-Sommerfeld) quantization exclusively. This development refers to the results of Sec. II A, since the equations derived in Sec. II B are already quantum mechanical or, as we have emphasized, can be so understood.

A. Quantization condition from the correspondence principle

In this time-honored method, we integrate the correspondence principle equation

$$w(n) = \frac{dE_n}{dn} , \qquad (3.1)$$

leading to $[w(n) \to w(E)]$

$$n = \int_0^{E(n)} \frac{dE}{w(E)} . \qquad (3.2)$$

The lower bound chosen implies a Bohr-Sommerfeld quantization rule.[9] This is the extent of the accuracy to which we shall work in this paper. To implement Eq. (3.2), we need $w(E)$, the frequency as a function of the energy. This is obtained from the equation

$$E(n) = \langle n \mid H \mid n \rangle = H_{n,\,v=0} \cong \frac{1}{T_n} \int_0^{T_n} dt\, W_{\mathrm{HF}}(t) , \qquad (3.3)$$

which is derived by the following steps: Evaluating $\langle n \mid H \mid n \rangle$ by the same sequence of approximations which lead to the TDHF equation itself, we simply recognize the result as the $v = 0$ Fourier component of $W_{\mathrm{HF}}(t)$, i.e., the time average of the nominally time-dependent Hartree-Fock energy, calculated with the density matrix $\rho_n(x_1 x_2 \mid t)$. Equation (3.3) defines E as a function of T and therefore w. The inversion of this relation provides us with the function $w(E)$.

The method just described has the superficial disadvantage that we must find periodic solutions starting from the ground state and going up in energy to the level in which we are interested.

B. Quantization condition from the variational principle

This approach will yield rather succinctly the quantization condition that has been presented repeatedly in the physics literature.[1-4] We have

$$\rho_n(x_1 x_2 \mid t) = \sum_h \phi_h(x_1 t)\phi_h^*(x_2 t) , \qquad (3.4)$$

where the sum is over the occupied orbitals, which are solutions of the Hartree-Fock equations

$$i\partial_t \phi_h(xt) = \int \mathscr{H}_n(x, x' \mid t)\phi_h(x't) . \qquad (3.5)$$

These equations (and their complex conjugates) can be derived from the usual Hamilton's principle,

$$\delta I_n = \delta \int_0^{T_n} \langle \Phi(t) \mid (i\partial_t - H) \mid \Phi(t) \rangle = 0 , \qquad (3.6)$$

where $\mid \Phi(t) \rangle$ is the Slater determinant composed of the orbitals $\phi_h(xt)$, and the variation is with respect to ϕ_h and ϕ_h^* subject to the boundary conditions

$$\delta\phi_h(x\,0) = \delta\phi_h(xT_n) = \delta T_n = 0 . \qquad (3.7)$$

It is more convenient for our purposes to utilize the principle of least action, namely

$$\Delta S_n = \Delta \int_0^{T_n} \langle \Phi(t) \mid i\partial_t \mid \Phi(t) \rangle = 0 . \qquad (3.8)$$

Here the variations satisfy the conditions

$$\delta\phi(x0)=[\delta\phi(xT_n)+\partial_t\phi_h(xT_n)\delta T_n]$$

$$=\delta\langle\Phi(t)\,|\,H\,|\,\Phi(t)\rangle=0 \ . \tag{3.9}$$

The consistency of the last condition follows from the constancy in time of the Hartree-Fock energy. The proof of (3.8) with the conditions (3.9) is the same as that to be found in any mechanics textbook[15] and will not be repeated. Recalling (3.3) and (3.6), we can write (3.8) in the form

$$\Delta S_n=\Delta(I_n+E_nT_n)=0 \ . \tag{3.10}$$

We apply this principle to the problem at hand by computing dS_n/dn. This can be written symbolically as a sum of two terms,

$$\frac{dS_n}{nd}=\frac{\Delta S_n}{\Delta n}+\frac{\partial S_n}{\partial n}=\frac{\partial S_n}{\partial n} \ , \tag{3.11}$$

where the first term (which is then dropped) is the contribution to the derivative from those terms which enter into the establishment of the variational principle $\Delta S_n=0$ and for this reason do not contribute. The quantity $\partial S_n/\partial n$ is then computed by varying only those quantities which both depend on n and remain unvaried in deriving (3.10). In the light of these remarks we note that $\partial I_n/\partial n=0$ and also $\partial T_n/\partial n=0$. Thus from (3.10) we have

$$\frac{dS_n}{dn}=\frac{dE_n}{dn}T_n=w(n)T_n=2\pi \ . \tag{3.12}$$

Thus we obtain the well-known condition

$$S_n=\int_0^{T_n}\langle\Phi\,|\,i\partial_t\,|\,\Phi\rangle$$

$$=\int_0^{T_n}dt\sum_h(\phi_h\,|\,i\partial_t\,|\,\phi_h)=2\pi n \ . \tag{3.13}$$

This condition may indeed be easier to apply in practice since, for a given n, it requires only identification of the appropriate periodic solution.

IV. DISCUSSION

In this paper we have presented two ideas. First, we have shown how periodic solutions of TDHF may be related to the spectrum of the system described. Such solutions may exist because the system exhibits a nearly decoupled, nearly harmonic collective subspace. This is certainly the most interesting possibility since it yields a relatively unambiguous physical picture.[6] In principle, we may also have a periodic solution emerge as a result of correspondence principle arguments applied to a bound motion. Since these arguments are most valid for large quantum numbers, in practice we are more likely to have to deal with multiply periodic solutions of substantial complexity. This point again seems to be borne out in practice,[5] where solutions have been obtained which apparently contain superposition of many different excitation branches. Even after the projection of given multipoles, the frequency distributions remain quite complex.

An interesting problem suggested by our considerations is how to choose initial values so as to obtain periodic solutions of a specified structure.

As a second contribution, we have described a derivation of the known quantization condition for periodic solutions which is certainly simpler and more direct than found in the previous (nuclear physics) literature. We have restricted ourselves to the Bohr-Sommerfeld level of accuracy, but the methods can be extended to include quantum corrections.[11]

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