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A B S T R A C T

A condition for the existence of a periodic TDHF trajectory of period T is derived. It takes a form very similar to the static H.F. equation and shows that associated to a periodic trajectory there is a static single particle hamiltonian which is a complicated functional of the time dependent density matrix. An explicit expansion for this functional is derived. We show that many properties of the static H.F. rest points are shared by periodic solutions.

K E Y W O R D A B S T R A C T

NUCLEAR STRUCTURE - Properties of periodic TDHF solutions. Expansion of monodromy matrix.

There is one striking difference between the meaning of the word self-consistency when applied to the static Hartree-Fock (HF) equations or to their time dependent counterparts. In the static case, the HF equations determine special points in the space of all Slater determinants (or density matrices). These are the rest points of the dynamical TDHF equations, and they are obtained, numerically, by a well known self consistent iteration scheme. This scheme, roughly speaking, starts with a density that is assumed to be close to the rest point. The HF hamiltonian for this density is calculated and diagonalized providing new eigenfunctions. A new density is constructed and the scheme is repeated until self-consistency, meaning that the input and output densities coincide, is achieved. By contrast, TDHF equations are evolution equations which for any initial density provide a sequence of densities (that we call a trajectory). Self consistency here means that the hamiltonian that propagates the solution at a given time depends on the density at that time.

The question then arises naturally as to whether special trajectories exist in the space of determinants. Rest points would be particular cases of such special trajectories.

Periodic solutions are known to play a prominent role in the study of hamiltonian systems with many degrees of freedom[1]. In particular they allow the study of semiclassical properties of its bound states[2]. Recently an extension of periodic orbit theory has also been successfully applied in field theory[3].

As the TDHF equations have been shown to be hamiltonian[4], it is natural to investigate its periodic solutions. These would be the candidates for the description of large amplitude collective motion within the TDHF approximation. Thus the special trajectories that we referred to above are the periodic ones [5]. The importance of periodic TDHF solutions has been recently stressed by several authors[6,7]

The purpose of this letter is to point out a condition for the existence of periodic solutions to the TDHF equations. This condition takes a form very similar to the static case and puts the important problem of the numerical search for periodic solutions on the same (albeit more complicated) level as the search for static Hartree-Fock rest points.

Consider the equations for the TDHF single particle wave functions

$$\left[h(\rho(t)) - i\frac{\partial}{\partial t} \right] |\varphi(t)\rangle = 0 \tag{1}$$

Here $h(\rho)$ is the usual HF hamiltonian

$$h(\rho) = t + \mathrm{tr}\,\rho v \tag{2}$$

where t is the kinetic energy and v is the antisymmetrized two-body interaction. $\rho(t)$ is the density matrix through which $h(\rho)$ becomes time dependent. Eq. (1) can be rewritten as

$$\left[h(\rho) - i\frac{\partial}{\partial t} \right] U(t) = 0 \quad , \quad U(0) = 1 \tag{3}$$

where U(t) is the single particle evolution operator. Self consistency is imposed with the requirement that

$$\rho(t) = U(t)\,\rho(0)\,U^{+}(t) \tag{4}$$

This requirement makes Eq.(3) non linear. To avoid problems with infinite matrices we will consider Eq.(1) or (3) in a single particle basis of large (but finite) dimension N. This basis will be in general a truncated set of eigenfunctions of some single particle operator. In particular, as is common in current TDHF calculations[8,9], it could be a set of position eigenfunctions on a discrete mesh. In this truncated basis all matrices have finite dimension and (3) becomes a system of first order ordinary differential equations. $U(t)$ is unitary while h and ρ are hermitian. Assume that a periodic solution for the density matrix exists with a period T

$$\rho(t+T) = \rho(t) \quad , \text{all } t \tag{5}$$

Then h is also a T-periodic matrix and for given $\rho(t)$, Eq.(3) becomes a linear differential system with periodic coefficients and $U(t)$ its fundamental matrix of solutions. Many theorems and properties are known for such systems[10]. In particular Floquet theorem states that the fundamental matrix of Eq.(3) can be decomposed as

$$U(t) = V(t)\, e^{-iMt} \tag{6}$$

where $V(t)$ is unitary and T-periodic and where M is a constant matrix which is easily shown to be hermitian. The initial condition on $U(t)$ implies $V(0)=1$ and therefore from the periodicity of V we deduce

$$U(T) = e^{-iMT} \tag{7}$$

$U(T)$ is the linear "mapping at a period" or monodromy matrix[10] for Eq.(3).

With $U(t)$ decomposed as in Eq.(6) the self consistency requirement (4) takes the form

$$\rho(t) = V(t)\, e^{-iMt} \rho(0)\, e^{iMt} V^{+}(t) \tag{8}$$

In general, ρ as calculated in Eq.(8) will not be T-periodic because M will mix in other frequencies incommensurable with T. This will not happen if the following condition is satisfied

$$[\dot{M}, \rho(0)] = 0 \tag{9}$$

This is the sought for condition for the existence of a T-periodic solution to the TDHF equations. Before seeing how it can be used, we give an explicit expression for M. To this purpose we use the continuous analogue of the Baker Hausdorff formula[11] or phase-expansion of the single particle evolution operator. If U(t) is written as

$$U(t) = e^{-i\Omega(t)} \tag{10}$$

then $\Omega(t)$ has the expansion

$$\Omega(t) = \int_0^t h(t_1)\,dt_1 - \frac{i}{2}\int_0^t dt_1 \int_0^{t_1} dt_2\,[h(t_1), h(t_2)] + \cdots \tag{11}$$

Higher terms in eq.(11) only involve multiple commutators of h(t) at different times and have been given explicitly in ref.(11). Comparison of (10) and (7) gives the explicit expansion of M

$$M = \frac{1}{T}\left\{ \int_0^T h(t_1)\,dt_1 - \frac{i}{2}\int_0^T dt_1 \int_0^{t_1} dt_2\,[h(t_1), h(t_2)] + \cdots \right\} \tag{12}$$

To the author's knowledge this formula for the computation of the logarithm of the monodromy matrix has not been reported before in the literature. M is a static single particle hamiltonian which is a complicated funtional of a T-periodic density. It will be denoted as $M[\rho_T(t)]$. In principle, it can be evaluated for any T-periodic trajectory and Eq.(9) selects the particular one which is also a solution of Eq.(3). Thus eq. (9) and (12) constitute the extension of the time-independent self-consistency problem of static HF to periodic time dependent solutions. In fact, for time independent HF solutions, when the periodic trajectory contracts to a rest point, the functional $M[\rho]$ reduces to $h(\rho)$ and condition (9) becomes the usual HF equation for the density matrix.

Eq.(9) can also be interpreted as an equation that selects the initial condition $\rho(0)$ so that it lies on a T-periodic trajectory. This is due to the fact that the equation for the density matrix (see Eq.16 below) is of first order in time and therefore the trajectory $\rho(t)$ is a unique function of the initial density and the time. Then the functional $M[\rho(t)]$, when computed along a solution to Eq.(16) with initial condition $\rho(0)$, becomes a function of $\rho(0)$, after all the time integrations have been performed. Thus Eq.(9) becomes $[M(\rho(0)), \rho(0)] = 0$ which is formally very similar to the static equation. Notice however that the function $M(\rho(0))$ is very complicated so that the problem is highly non linear. An effective solution can only be achieved by successive iterations.

Just as in the time independent case, Eq.(9) is best exploited in the basis which simultaneously diagonalizes M and $\rho(0)$. In this basis Eq.(1) and (4) take the form

$$\left[h(\rho) - i\frac{\partial}{\partial t} \right] |\varphi_n\rangle = \alpha_n |\varphi_n\rangle \tag{13}$$

$$\rho(t) = \sum_{n_{occ}}' |\varphi_n(t)\rangle\langle\varphi_n(t)| \tag{14}$$

where α_m are the eigenvalues of M and n_{occ} indicates the occupation pattern specified by the diagonal $\rho(0)$. The boundary condition for Eq.(13) is .

$$|\varphi_m(t+T)\rangle = |\varphi_m(t)\rangle \tag{15}$$

Eq. (13) with (15) have been recently considered in the context of a functional integral approach[6)]. There the eigenvalues α_n have been shown to play a role in the semiclassical quantization of a TDHF periodic trajectory.

The eigenvalues α_m are the stability angles, or characteristic exponents of Eq.(3). They are defined modulo $2\pi/T$ and, because M is hermitian, they are always real. They are associated to the periodic trajectory as a whole and not to a particular point on it. They are therefore the natural extension of the concept of single particle energies to a situation where a large amplitude collective oscillation is present. The determination of the α_m is probably best done through an iterative solution of Eq. (13) with periodic the boundary conditions (15). This is an intricate numerical problem and valuable physical insight into it can be obtained through a study of the static hamiltonian M in the x-representation (range, depth, diffuseness, non-locality, etc). The expansion (12) provides a basis for such a study.

Eq.(13) is an eigenvalue problem which, because of (14) has to be solved by an iteration scheme entirely analogous to the time independent one. Thus, one guesses an initial T-periodic density $\rho^{(o)}(t)$ and solves iteratively Eq.(13) until a self consistent time dependent density is obtained. Just as in the static HF scheme, no guarantee exists that the procedure will converge, or that for a given period T, a self consistent T-periodic trajectory exists at all. However, if it does and if the initial guess $\rho^{(o)}(t)$ is sufficiently close to it, we can expect this procedure to work.

It is important at this point to remark that the time evolution of the single particles is not unique. Any time dependent transformation that leaves the density matrix invariant (namely linear combinations of occupied or unoccupied orbitals) will yield very different s.p.w.f. while leading to the same trajectory $\rho(t)$. Eq.(1) selects a particular combination but it is not invariant under such a transformation. Thus the matrix M, toghether its eigenvalues, depends on with s.p. evolution equation we choose to solve and is not uniquely associated with a periodic trajectory as specified by $\rho(t)$. Again, this arbitrariness in the definition of the single particle hamiltonian is also present in the familiar static case.

Althrough the α_M were called stability angles, it should be clear that they are not related to the stability properties of the periodic orbit. This is already apparent for rest points, whose stability is related to RPA frequencies and not to single particle energies. The detailed stability analysis of periodic trajectories is outside the scope of this work and will be reported elsewhere. We can however give a brief argument showing that quantities similar to RPA frequencies will be associated to a trajectory and will determine its stability properties.

Consider the TDHF equation for the density matrix

$$i\dot{\rho} = [h(\rho), \rho] \tag{16}$$

If a T-periodic solution $\rho(t)$ is known we look for nearby solutions $\rho'(t) = \rho(t) + \delta\rho(t)$. After linearizing, the resulting equation for $\delta\rho(t)$ is

$$i\frac{d}{dt}\delta\rho = [h(\rho), \delta\rho] + [\mathrm{tr}\, v\,\delta\rho, \rho] \tag{17}$$

This is a linear equation with periodic coefficients for $\delta\rho(t)$. Again Floquet's theorem can be applied and solutions can be looked for in the form $\delta\rho = \delta\rho_n(t)\exp(-i\omega_n t)$ where $\delta\rho_n(t)$ is T-periodic and ω_n are constants. The equations for $\delta\rho_n$ are

$$i\frac{d}{dt}\delta\rho_n - [h(\rho),\delta\rho_n] - [\mathrm{tr}V\delta\rho_n,\rho] = -\omega_n\delta\rho_n \tag{18}$$

and they have to be solved with periodic boundary conditions

$$\delta\rho_n(t+T) = \delta\rho_n(t) \tag{19}$$

Eq.(18) generalizes the R.P.A. equation for a periodic solution and reduces to the familiar form in the static limit. Notice that ω_n are a characteristic of the whole periodic trajectory and can be quite different from local R.P.A. frequencies. In contrast to (1), the evolution of $\delta\rho(t)$ is governed by a non hermitian matrix and therefore it can occur that some of the frequencies become imaginary. In that case the periodic solution is unstable.

Several questions need further investigation. First and foremost is the convergence of expansion (12) in same small parameter so that the static field can be effectively computed. Next are the numerical problems involved in the iterative solution of Eq.(13). The latter have been addressed to briefly in ref.(6). From this investigation it seems that what for rest points was an algebraic diagonalization problem, for periodic trajectories becomes the computation of the monodromy matrix of a system of differential equations with periodic coefficients. Although numerical methods exist for this computation[10)], they would have to be adapted to the TDHF problem.

In conclusion we have shown that associated with a periodic solution to the TDHF equations we have two sets of constant numbers which generalize the notions of single particle energies and RPA frequencies and which reduce to the usual quantities when the periodic trajectory reduces to a rest point. The periodic trajectory itself is determined by a self consistent condition involving a static field which also generalizes the HF equation .

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