A Numerical Study on the Structure Change of Collective Motions

Yukio HASHIMOTO, Kazuo IWASAWA,* Fumihiko SAKATA* and Akio NARUI

Institute of Physics, University of Tsukuba, Tsukuba 305
*Institute for Nuclear Study, University of Tokyo, Tanashi 188

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With the aim of investigating the structure of the TDHF symplectic manifold, the relation between the TDHF trajectories and the collective potential energy curves is studied. It is shown that a structural change of the collective motion takes place when the number of local minima connected with the corresponding trajectory varies. A new numerical method for reaching the local minima affecting a given trajectory is illustrated within a simple soluble model. Its feasibility for studying the structural change of the collective motion is shown by applying it to a more realistic case with a simple density dependent effective interaction.

§ 1. Introduction

It has been one of the longstanding problems in both nuclear structure and nuclear reaction physics whether the adiabatic single-particle states or the diabatic ones are more appropriate for describing large-amplitude collective motion. This problem is ultimately related to the question of what kind of single-particle configuration remains to be a constant of motion (or good quantum number) during the development of the collective motion. Therefore, their proper physical meaning ought to be clarified by studying the exceedingly rich structure of the time-dependent Hartree-Fock (TDHF) symplectic-manifold, where the nonlinear effects in a finite many-fermion system are expected to play a decisive role. According to recent remarkable progress in the general theory of the nonlinear dynamical system, e.g., the order-to-chaos transition dynamics, it has been clarified that the phase space is filled with various types of motion caused by nonlinear interactions, which are not expected from simple physical intuition, but are only explored through numerical simulation. An analytic understanding of the nonlinear phenomena, i.e., the development of the nonlinear theory can be well achieved, only after the complicated phase space structure has been explored numerically.

The aim of the present paper is to develop a new algorithm for studying the complicated structure of the TDHF-manifold, by going one step further from our previous work. In the previous work, we restricted ourselves to the structure of the TDHF coordinate space, i.e., the shape of the potential energy surface (PES) in the multi-dimensional coordinate space. In the practical numerical method, it is well known that the constrained (C-)HF equation is more feasible than the HF equation in searching for many local minima satisfying the HF condition. Conventionally, the CHF equation has been solved numerically by using the gradient method, which usually reaches the most energetically favorable state for a given constraining condition, and ends up with the adiabatic collective potential. It may be associated with a rather sudden change of the configuration as well as an abrupt change in the
structure of the single-particle orbitals. On the other hand, another potential, called the diabatic collective potential, has been introduced, which is defined under the following assumption: the structure of the single-particle orbitals and the configuration are kept unchanged regardless of the magnitude of the constraining value. Since the nucleus is a self-sustained system, however, the structure of the single-particle orbitals depends on the constraining values due to the self-consistency of the mean-field. To introduce the diabatic single-particle orbitals, one usually applies a practical method so as to eliminate the “virtual interaction”, which induces a relatively large structural change of the single-particle orbitals. Although there is much phenomenological support for introducing the diabatic basis, there certainly exists some ambiguity in defining the virtual interaction to be eliminated.

In order to study an applicability and a limitation of both the adiabatic and diabatic single-particle orbitals, it is desirable to explore the structure of the TDHF manifold, where two types of single-particle orbitals show quite different properties. Aiming at studying what happens in this region, and finding out many other HP points usually not accessible by the conventional numerical method, we proposed the reference state (RS) method by exploiting the fact that the CHF solutions always constitute many differentiable CHF-lines in the TDHF coordinate space, and every HF point rests on one of these lines. In Fig. 1(a), an example of the CHF-lines projected onto the constraining collective subspace (the quadruple deformation variable) is shown. What is observed in Fig. 1 is that the main components of the wave functions on the curves (i) and (iii) are interchanged, as the magnitude of the deformations.

![Figure 1](https://academic.oup.com/ptp/article-abstract/95/5/883/1866518)

Fig. 1. (a) Continuous CHF lines. The lowest line i) passes through the ground state $|\phi_0\rangle$. The dense calculated points near $q=0.02$ and $q=-0.05$ indicate an abrupt character change occurring in line i). To illustrate “diabatic line” having no abrupt change, the dashed lines are drawn by hand. (b) The corresponding single-particle energy levels. Solid lines are results from the global configuration dictated (GCD) method, and dashed lines are from the local configuration dictated (LCD) method. The filled and open circles represent the occupied and unoccupied states, respectively. (Borrowed from Ref. 4)).
tion changes from prolate to oblate. This structural change is numerically detected in the RS-method, because the increment of the deformation used in the calculation is chosen numerically in such a way that the squared overlap between two adjacent CHF states belonging to the same CHF-line should not be less than 0.9. This condition guarantees the continuity property of the CHF-line. Actually, the numerical results turned out to be the same as in the calculation of Fig. 1 when one applies the more severe condition 0.99 instead of 0.9. As is seen in Fig. 1(a), the calculated points become dense near \( q = 0.02 \) and \( q = -0.05 \), indicating a rather sudden change of the single-particle wave functions constituting the CHF state. This suggests that the configuration change is taking place rather abruptly near the dense calculated-point region, in comparison with the other part of the CHF-line. It is also seen that this character change along the CHF-line is closely related with the single-particle level crossings (Fig. 1(b)). Applying the conventional phenomenological method of introducing the diabatic basis, in Fig. 1(a), one may draw the "diabatic-lines", which start from the observed dense calculated points on the CHF-lines.

In order to explore the basic issue regarding the adiabatic single-particle states vs. the diabatic ones, and an effect of the structural change in the CHF-line on the collective excitation mode, one must study the properties of the TDHF trajectories, whose initial condition is set on the various points on a given CHF line. For this purpose, it turns out to be inevitable to develop a new numerical method appropriate for clarifying the structural change of the TDHF trajectory, which is running in a region where more than two different CHF lines come close to one another.

Showing the basic idea of the new numerical method, in § 2, we adopt the simple three-level model in Ref. 7). By projecting the CHF-lines as well as the TDHF-trajectories onto the collective subspace, we discuss the relation between them. The structural change of the TDHF trajectory is investigated by means of a newly developed method, which intends to find a set of various local minimum points affecting the trajectory. In § 3, the feasibility of the new method discussed in § 2 is illustrated by applying it to a more realistic case with a density dependent effective interaction. Section 4 is devoted to summary and discussion.

§ 2. Reference state method for the TDHF trajectory
—— SU(3) model case ——

2.1. The model Hamiltonian and TDHF equations

In this section, we discuss what one can learn from the TDHF trajectory by using a simple soluble model. Let us start with brief recapitulation of the simple SU(3) model introduced in Ref. 7). The model consists of three single-particle levels with the same \( N \)-fold degeneracy. The Hamiltonian contains the single-particle energy terms satisfying \( \varepsilon_0 < \varepsilon_1 < \varepsilon_2 \) and two-body interaction terms:

\[
\hat{H} = \hat{H}_0 + \hat{H}_v + \hat{H}_Y,
\]

\[
\hat{H}_0 = \varepsilon_0 \hat{K}_{00} + \varepsilon_1 \hat{K}_{11} + \varepsilon_2 \hat{K}_{22},
\]

\[
\hat{H}_v = \frac{V_1}{2} (\hat{K}_{10} \hat{K}_{01} + \text{h.c.}) + \frac{V_2}{2} (\hat{K}_{20} \hat{K}_{02} + \text{h.c.}),
\]

\[
\hat{H}_Y = \alpha \hat{K}_{10} \hat{K}_{01} + \beta \hat{K}_{20} \hat{K}_{02} + \gamma (\hat{K}_{10} \hat{K}_{01} + \text{h.c.}) + \text{h.c.},
\]

where \( \alpha, \beta, \gamma \) are coupling constants. The energy eigenvalues and eigenvectors of the Hamiltonian \( \hat{H}_0 \) are known analytically. The eigenvalues are:

\[
\lambda = \varepsilon_0, \quad \lambda = \varepsilon_1, \quad \lambda = \varepsilon_2.
\]

The eigenvectors are:

\[
|\Psi_0\rangle = |\varepsilon_0\rangle, \quad |\Psi_1\rangle = |\varepsilon_1\rangle, \quad |\Psi_2\rangle = |\varepsilon_2\rangle.
\]

The TDHF trajectory is defined by the time-dependent wave function:

\[
|\Psi(t)\rangle = |\Psi_0\rangle e^{-iH_0 t} \left( e^{H_0 t} e^{H_v t} e^{H_Y t} - 1 \right) |\Psi_0\rangle.
\]

The TDHF trajectory is then given by the time evolution of the wave function.

The reference state method is introduced to clarify the structural change of the TDHF trajectory. The reference state method is a numerical method for solving the TDHF equation. The reference state is chosen to be the ground state of the Hamiltonian \( \hat{H}_0 \). The TDHF trajectory is then approximated by the time evolution of the wave function in the reference state.

The reference state method is known to be effective for studying the collective excitations. The reference state method is also known to be effective for studying the structural change of the TDHF trajectory. The reference state method is known to be effective for studying the collective excitations. The reference state method is also known to be effective for studying the structural change of the TDHF trajectory.
\[ \hat{H}_V = V_0(\hat{K}_{10}(\hat{K}_{11} + \hat{K}_{22}) + \text{h.c.}) + V_4(\hat{K}_{10}(\hat{K}_{12} + \hat{K}_{21}) + \text{h.c.}) + V_0(\hat{K}_{20}(\hat{K}_{11} + \hat{K}_{22}) + \text{h.c.}) + V_6(\hat{K}_{20}(\hat{K}_{12} + \hat{K}_{21}) + \text{h.c.}), \]

where the operator \( \hat{K}_0 \) is a one-body operator defined as
\[ \hat{K}_0 = \sum_{m=1}^{N} \hat{C}_{im} \hat{C}^*_{jm}. \]

The general time-dependent Slater-determinant state |\( \phi(t) \rangle \) for the \( N \)-particle system is given by
\[ |\phi(t)\rangle = e^{\hat{F}(t)} |\phi_0\rangle, \quad \hat{F}(t) = \sum_{i=1}^{2}(f_i(t)\hat{K}_0 - \text{h.c.}), \]

where \( |\phi_0\rangle \) is the HF state
\[ |\phi_0\rangle = \prod_{m=1}^{N} \hat{C}_{im} |0\rangle, \quad \hat{C}_{im}|0\rangle = 0, \quad (i=0, 1, 2) \]

satisfying the HF equation
\[ \partial \langle \phi_0 | \hat{H} | \phi_0 \rangle = 0. \]

The TDHF trajectory is determined by the canonical equations of motion
\[ i\hbar \frac{\partial C_j}{\partial t} = \frac{\partial \mathcal{H}}{\partial C^*_j} \quad \text{and} \quad \text{C. C.,} \quad j=1, 2, \quad (2·6) \]
\[ \mathcal{H} = \langle \phi(f) | \hat{H} | \phi(f) \rangle, \]

where a set of canonical variables \((C^*_j, C_j; j=1, 2)\) is introduced through the transformation \((f^*_j, f_j)\rightarrow(C^*_j, C_j), \)
\[ C_j = \sqrt{N}f_j \sin \frac{\sqrt{\sum_{i=1}^{2} f^*_i f_i}}{\sqrt{\sum_{i=1}^{2} f^*_i f_i}} \quad \text{and} \quad \text{C. C.,} \quad j=1, 2. \]

Using a set of real variables \((x_j, p_j; j=1, 2)\) defined through
\[ x_j = (C^*_j + C_j)/\sqrt{2}, \quad p_j = i(C^*_j - C_j)/\sqrt{2}, \quad j=1, 2, \]

the canonical equations of motion in Eq. (2·6) are rewritten as
\[ \dot{x}_j = \frac{\partial \mathcal{H}}{\partial p_j}, \quad \dot{p}_j = -\frac{\partial \mathcal{H}}{\partial x_j}, \quad j=1, 2. \]

In this model case, we use the convention \( \hbar = 1. \) The set of canonical variables \((x_j, p_j; j=1, 2)\) describes the TDHF manifold and the coordinate space \((x_1, x_2)\) is called the TDHF coordinate space. The two-dimensional PES \( V(x_1, x_2) \) is defined as
\[ V(x_1, x_2) = \langle \phi(x) | \hat{H} | \phi(x) \rangle, \]
\[ |\phi(x)\rangle = |\phi(x_1, x_2, p_1 = p_2 = 0)\rangle. \]

This is shown in Fig. 2.
The general constraining one-body operator is given by \(^7\)

\[
\tilde{Q} = Q_{1x}(\tilde{K}_{10} + \tilde{K}_{01}) + Q_{1y}(\tilde{K}_{20} + \tilde{K}_{02})
+ Q_{2x}\tilde{K}_{11} + Q_{2y}\tilde{K}_{22} + Q_3\tilde{K}_{00} + Q_4(\tilde{K}_{21} + \tilde{K}_{12}).
\] (2.11)

By means of the function defined through

\[
q(x_1, x_2) = \langle \phi(x) | \tilde{Q} | \phi(x) \rangle,
\] (2.12)

each point on the TDHF coordinate space \(\{x_1, x_2\}\) is mapped onto the constraining coordinate space \(\{q\}\), which will be called the collective subspace. The CHF equation is given by

\[
\delta q | \hat{H} - \lambda \tilde{Q} | q \rangle = 0, \quad q = \langle q | \tilde{Q} | q \rangle,
\]

\[
| q \rangle = | \phi(x_1(q), x_2(q)) \rangle,
\] (2.13)

whose solution is also shown in Fig. 2. As is seen from Fig. 2, there are more than two continuous CHF lines in the TDHF coordinate space, and there exists some region where more than two CHF states coexist for a given constraining condition. The parameters used for the Hamiltonian (2.1) are: \(N=4, \varepsilon_0=0, \varepsilon_1=16.4, \varepsilon_2=18, V_1 = V_2=-16/3, V_3=-4/15, V_4=-2/15, V_5=0, V_6=-8/3\). The parameters in the constraining operator \(\tilde{Q}\) are: \(Q_{1x}=1, Q_{1y}=1/5, Q_{2x}=Q_{2y}=2, Q_3=Q_4=0\).
2.2. TDHF trajectories and CHF lines

By projecting the continuous CHF lines onto the collective subspace through Eq. (2·12), one obtains many continuous collective PES for a given \( q \). On the other hand, the \textit{adiabatic} collective PES is introduced by connecting the pieces of the continuous collective PESs by using such a condition that the energy should be minimum for any given value of \( q \).

Since we are interested in the relation between the collective motion and the

![Fig. 3](https://academic.oup.com/ptp/article-abstract/95/5/883/1866518)

**Fig. 3.** (a) Potential energy curves along the branches A(full curve) and B(dashed curve) in Fig. 2 versus expectation value \( q = \langle \hat{Q} \rangle \). The dash-dotted curve represents the adiabatic potential curve. The \( V-q \) plots of the typical TDHF trajectories around the minimum \( \phi_i \) are represented by line-segments labelled as i)~iii). The trajectories are shown in (b)~(d), in which filled circles denote the local minimum \( \phi_i \).
adiabatic and/or diabatic collective PESs in the collective subspace, the initial conditions of the trajectories are chosen at various points on the CHF lines. The calculated results of the TDHF trajectories are shown in Figs. 3~5. In these figures, we show the adiabatic and continuous collective PESs (called the "V-q plane"), as well as the projected TDHF trajectories around the HF points φ₁ and φ₂ onto the collective subspace.

When the energy of the TDHF trajectory around the point φ₁ is small and below that of another local minimum point φ₂ (i.e., case i) in Fig. 3(a)), the continuous collective PES, which limits the amplitude of the projected trajectory, is identical with the adiabatic collective PES. In this case, the conventional picture where the collec-

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![Diagram](https://example.com/diagram.png)

**Fig. 4.** (a)~(d) As in Fig. 3 but for the TDHF trajectories around the minimum φ₂. In (a), dashed curve is branch A and full curve is branch B in Fig. 2. In (b) ~ (d), filled circles denote the local minimum φ₂.
tive motion of the system is controlled by the adiabatic collective PES may be valid for describing the collective dynamics of the system.

On the other hand, when the energy of the TDHF trajectory is above that of another local minimum point $\phi_2$ (i.e., cases ii) and iii) in Fig. 3(a)), the conventional adiabatic picture no longer holds. The smaller limit $q$ of the projected TDHF trajectory is not on the adiabatic collective PES, which is a part of the projected CHF line characterized by the local minimum point $\phi_2$, but on the projected CHF line passing through $\phi_1$. In this situation, it is clearly seen that the TDHF trajectory is not controlled by the adiabatic collective PES, but closely related to the continuous collective PES, along which a change of the single-particle configuration remains minimum as the constraint value changes. The TDHF trajectories on the TDHF coordinate space are shown in Figs. 3(b)~(d).

In Fig. 4, one may observe the same situation for the TDHF trajectories, which are restricted around the local minimum point $\phi_2$. The projected trajectory, whose

![Fig. 5.](image-url)

(a) As in Fig. 3(a) but the TDHF trajectory has larger excitation energy. It starts from a point on branch A (full curve). The dashed curve is branch B in Fig. 2. (b) Poincaré map of the trajectory. (c) Projection of the trajectory onto the TDHF coordinate space.
initial condition is set at some point on the CHF line characterized by \( \phi_2 \), is also limited by the continuous collective PES. Though the initial condition of the trajectories is alternatively regarded to be put on the adiabatic collective PES, the trajectories do not reach the other side of the adiabatic collective PES. The TDHF trajectories on the TDHF coordinate space are shown in Figs. 4(b)~(d).

Thus the conventional viewpoint based on the adiabatic collective PES is not appropriate for understanding the dynamical behavior of the TDHF trajectories in Fig. 4. However, it is important to note that the major feature of the collective trajectory starting from some point on the CHF line is well described by the collective variables alone, because it is connected with only one potential minimum, and the main component of the trajectory is represented by the constraining coordinate \( q \) alone.

When the energy of the TDHF trajectory becomes sufficiently large (Fig. 5), the projected trajectory seems to be limited by the adiabatic collective PES, and controlled by it. However, the situation is not so simple. The TDHF trajectory displays an irregular motion in the TDHF manifold. Its pattern is complicated and looks even chaotic in the Poincaré section map illustrated in Fig. 5(b). In Fig. 5(c), the situation can be clearly seen when the TDHF trajectory is displayed on the TDHF coordinate space. In this coordinate space, the trajectory seems to cover densely a wide triangular area, which is allowed for a given energy. In this energy region, a single collective PES is not appropriate to describe the complicated behavior of the TDHF trajectory, no matter whether it is adiabatic or continuous collective. What is important in the present case is to recognize that the TDHF trajectory is not described by the collective variable alone, but by introducing an additional degree of freedom which can distinguish different potential minima.

2.3. HF points affecting the TDHF trajectory

---Trajectory referred method---

In the previous subsection, it was shown that the projected CHF lines on the collective subspace give many continuous collective PESs. By solving the TDHF equation, it was also shown that the collective motion starting from a series of consecutive points on the CHF lines undergoes structural changes when the number of local minima connected with the trajectory changes. The structural change indicates the necessity of additional degrees of freedom so as to identify the different local minima, in addition to the constraining collective variables. Consequently, it is desirable to develop a new numerical method of finding out many local minima which affect a given trajectory. Since one possible way may be provided by applying the RS method to an arbitrary point on the TDHF trajectory, let us recapitulate the method in a form appropriate for the present purpose:

1. Choose the single-Slater determinant \( |\phi^{(\alpha=0)}\rangle \), which is the real part of the TDHF state at an arbitrary time. The state \( |\phi^{(\alpha=0)}\rangle \) is represented as

\[
\begin{pmatrix}
\beta x_2 \\
\beta x_1 \\
2\beta y
\end{pmatrix},
\]

(2.14)
where \( \gamma = \sqrt{(N - (x_1^2 + x_2^2 ))/2} \), \( \beta = 1/(2N) \). Both \( x_1 \) and \( x_2 \) are given by the TDHF equation (2.9). Regarding \( | \phi^{(n=0)} \rangle \) as a reference state (RS) \( | \phi_{RS} \rangle \), we start the following iterative process.

2. Calculate the density \( \rho^{(n)} \) and the one-body Hamiltonian \( h[\rho^{(n)}] \) by using \( | \phi^{(n)} \rangle \). The one-body Hamiltonian \( h[\rho^{(n)}] \) is given as a matrix \( h_{ij} \) by the relation

\[
h_{ij} = \frac{\partial V}{\partial \rho_{ij}},
\]

(2.15)

where \( V \) is given in Eq. (2.10). Here, the density matrix \( \rho_{ij} \) is defined as

\[
\rho = \frac{1}{2} \begin{pmatrix} x_2^2 & x_2 x_1 & \gamma x_2 \\
x_1 x_2 & x_1^2 & \gamma x_1 \\
\gamma x_2 & \gamma x_1 & 4 \gamma^2 \end{pmatrix}.
\]

(2.16)

After diagonalizing the single-particle Hamiltonian \( h[\rho^{(n)}] \), a new set of single-particle states \( | \phi_i^{(n+1)} \rangle; i = 1, 2, 3 \) is obtained.

3. Find a hole state \( | \phi_i^{(n+1)} \rangle \), which has the largest overlap with that in the reference state \( | \phi_{RS,i=1}^{(n+1)} \rangle \). Here, the occupied single-particle state in the RS is the only one in the present model, and is denoted by \( | \phi_{RS,i=1} \rangle \). This is called the maximum overlap condition (MOC).\(^4\) Thus, the new density \( \rho^{(n+1)} \) and the new one-body Hamiltonian \( h[\rho^{(n+1)}] \) are obtained by using the new hole state \( | \phi_i^{(n+1)} \rangle \) satisfying the MOC.

4. The above steps 2 and 3 are repeated until a self-consistency between the eigenstate \( | \phi_i^{(n)} \rangle \) and the one-body Hamiltonian \( h[\rho^{(n)}] \) is completed.

As is easily recognized in the above iterative process, one may reach the HF state which is located at the nearest point to the reference state \( | \phi^{(n=0)} \rangle \). Since the real part of the TDHF state is taken as a reference state, the above numerical procedure will be called the trajectory referred (TR) method.

Typical results obtained from the above numerical method are shown in Figs. 6~8. In these figures, the iterative processes starting from various points on the TDHF trajectory are shown together with the resulting stationary points in the collective subspace \( \{q\} \).

In Figs. 6 and 7, we show the case where the excitation energy is rather small, and the TDHF trajectory is restricted in the neighborhood of the local minimum point. In this case, the above method connects the reference points (states) on the trajectory with the corresponding local minimum point. From the figures, it can be seen that each point on the TDHF trajectories is characterized by only one basic stationary mean-field, i.e., local minimum point \( \phi_1 \) or \( \phi_2 \). This means that the single-particle configuration corresponding to the local minimum point remains to be the main component in the time-dependent state specified by \( (x_i(t), p_i(t)) \) in the TDHF manifold. For these cases, the projected CHF lines onto the collective subspace have the meaning of the collective PES as long as the excitation energy of the trajectory is not too high.

On the other hand, in Fig. 8, we illustrate the case where the excitation energy is
Fig. 6. (a) Iteration processes (full curves) of the TR method from sample points on the TDHF trajectory (dashed curve) in Fig. 3(c). The dotted curve is curve A in Fig. 2. (b) Integration time of the TDHF trajectory versus resulting points of the iteration processes in (a) represented by the expectation values \( q = \langle \mathcal{Q} \rangle \) at the points. The resulting points are \( \phi_i \) in Fig. 2. The full curve represents the expectation values \( \langle \phi(f)|\mathcal{Q}|\phi(f)\rangle \) of the constraining operator \( \mathcal{Q} \) in terms of the TDHF state \(|\phi(f)\rangle\).

Fig. 7. (a) and (b) As in Fig. 6 but for the TDHF trajectory (dashed curve) in Fig. 4(b). The dotted curve is branch B in Fig. 2. The resulting points are \( \phi_i \).

high enough and the TDHF trajectory covers a much wider area of the TDHF manifold. In this case, the trajectory is connected with three different minimum points. Though the trajectory is irregular (even chaotic) in the TDHF manifold, our method can find three different stable mean-fields, which are embedded in the “stochastic sea”. In the figures, we can see that the trajectory visits three different areas specified by the local minimum points in an irregular order and stays there for an indefinite period.

In this way, the method stated above clarifies one aspect of the character changes of the collective motion as it develops from a small amplitude to a large one. Here, the character change in the trajectory is represented by the set of local minimum
point(s) obtained by the method. When the excitation energy of the TDHF trajectory is small, the method picks up only one minimum point irrespective of the starting point on the TDHF trajectory. As the excitation energy becomes high, the method gives several local minimum points, which affect the trajectory. Since every point on the TDHF trajectory is connected with a certain local minimum point, the points on the TDHF trajectory can be classified into several groups in terms of these local minimum points, with which they are connected, even if the trajectory displays irregular patterns in the phase space.

§ 3. Properties of the TDHF trajectory
—— A case with the density dependent Hamiltonian ——

3.1. High-lying Hartree-Fock states and CHF lines

In the previous section, it was shown that the collective PES does not necessarily yield adequate information when it develops into the large amplitude region. This situation is expected to occur when the TDHF trajectory is under the influence of more than two local minima, and when many CHF lines come close to each other. Although the quantum mechanically interesting TDHF trajectories may be the closed orbits, it is decisive to know a set of new coordinates which can distinguish many local minima connected with the collective TDHF trajectories. It is the objective of the present section to study whether the method proposed in the previous section is also applicable for the realistic case.

Let us apply the new numerical method to a more realistic case with the density dependent effective interaction. The single-particle Hamiltonian is chosen to have the following form:8

\[
h[\rho(r)] = -\frac{\hbar^2}{2m} \nabla^2 + W[\rho(r)],
\]  

(3.1)
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\[ W[\rho(r)] = 2a_2\rho(r) + 3a_3\rho^2(r) - 2a_s\nabla^2\rho(r), \]

where \( \rho(r) \) is the nucleon density,

\[ \rho(r) = 4\sum_{j=1}^{A'} p_j(r) \phi_j(r), \quad A' = A/4, \tag{3·2} \]

and \( a_2, a_3 \) and \( a_s \) are constants. Here, \( \phi_j(r) \) is a single-particle wave function and \( A \) is the total number of nucleons. For simplicity, we neglect the spin and isospin degrees of freedom of the nucleon and consider only the spatial part of the single-particle wave function \( \phi_j(r) \) \( (j=1, \ldots, A') \). This form of the single-particle Hamiltonian has been used in Ref. 8). The total energy corresponding to the single-particle Hamiltonian is

\[ E_{\text{total}} = \int dr^3 \left( \frac{\hbar^2}{2m} |\nabla \phi_j(r)|^2 + a_2\rho^2(r) + a_3\rho^3(r) + a_s(\nabla^2 \rho(r))^2 \right). \tag{3·3} \]

Using the single-particle Hamiltonian in Eq. (3·1), one can calculate both the HF ground state and the high-lying HF states in the same way as has been proposed in Ref. 4). The procedure to find the high-lying HF states in Ref. 4) is simply recapitulated as follows; having obtained the HF state \( |\phi_0\rangle \) (e.g., the HF ground state), one may construct a single-Slater determinant \( |\phi_{ph}\rangle \) which has a many-particle many-hole structure with respect to \( |\phi_0\rangle \), i.e.,

\[ |\phi_{ph}\rangle = \prod_i (\hat{C}_p^\dagger \hat{C}_n) |\phi_0\rangle, \tag{3·4} \]

where \( \hat{C}_p, (\hat{C}_n) \) is a Fermion operator creating a particle (hole) state with the quantum number \( \rho_i(h_i) \) with respect to the HF state \( |\phi_0\rangle \). One may then apply the RS-method with MOC discussed in § 2.3, by choosing \( |\phi_{ph}\rangle \) as a reference state \( |\phi_{RS}\rangle \). Our numerical calculations have been carried out by using the set of parameters \( A = 80, a_2 = -408.4(\text{MeV} \cdot \text{fm}^3), a_3 = 1079.4(\text{MeV} \cdot \text{fm}^6) \) and \( a_s = 67.7(\text{MeV} \cdot \text{fm}^5) \). In this paper, we restrict ourselves to the case with axial symmetry and reflection symmetry. The \( z \)-axis projection \( (\Omega) \) of the nucleon angular momentum and the parity \( (\pi) \) of the nucleon wave function are good quantum numbers.

In Fig. 9, several high-lying HF states are shown together with the HF ground state \( |\phi_0\rangle \). In order to obtain the CHF line, which passes through a given HF point, the local configuration dictated (LCD) method\(^9\) has been used.

3.2. The TDHF trajectory and the trajectory referred method

The TDHF equation with the single-particle Hamiltonian in Eq. (3·1) is

\[ \text{Fig. 9. Continuous CHF lines with high-lying HF points (labelled 1 8).} \]
given as
\[ i\hbar \frac{\partial}{\partial t} \psi_j(r, t) = h[p(r, t)] \psi_j(r, t), \quad j = 1, \cdots, A', \quad (3.5) \]
\[ \rho(r, t) = 4 \sum_{(\text{occupied})} \psi_j^*(r, t) \psi_j(r, t), \]
where the nucleon density \( \rho(r, t) \) is constructed by using the occupied single-particle wave functions \( \psi_j(r, t) \). The occupied states are specified by the initial conditions at \( t = 0 \).

The solution of the TDHF equation (3.5) is formally expressed as\(^9\)
\[ \psi_j(r, t) = T \exp \left[ -\frac{i}{\hbar} \int_0^t h[p(r, \tau)] d\tau \right] \psi_j(r, 0), \quad (3.6) \]
where \( T \) is a time-ordering operator. In the practical numerical calculation, time is divided into discrete steps, and the formal solution in Eq. (3.6) is used to propagate a wave function at time \( t_n \) \((n = 0, 1, 2, \cdots)\) into that at \( t_{n+1} \),
\[ \psi_j(r, t_{n+1}) = \exp \left[ -\frac{i}{\hbar} \cdot \Delta t \cdot \hbar[p_{n+1}, p_n] \right] \psi_j(r, t_n), \quad (3.7) \]
where \( \hbar \) is a one-body Hamiltonian introduced for keeping the total energy constant,\(^10\) and \( \Delta t \) is a time step of integration which is taken to be \( 10^{-24} \) (second) in our calculations. The Hamiltonian \( \hbar \) is made of the nucleon density \( \rho_{n+1} \equiv \rho(r, t_{n+1}) \) at \( t_{n+1} \) and \( \rho_n \equiv \rho(r, t_n) \) at \( t_n \). In the present case, \( \hbar \) has the following form,
\[ \hbar = -\frac{\hbar^2}{2m} \mathbf{v}^2 + a_2(\rho_{n+1} + \rho_n) + a_3(\rho_{n+1}^2 + \rho_{n+1} \rho_n + \rho_n^2) - a_4 \mathbf{v}^2(\rho_{n+1} + \rho_n). \quad (3.8) \]

The exponential function in Eq. (3.7) is approximated by the power series expansion
\[ \exp \left( -\frac{i}{\hbar} \cdot \Delta t \cdot \hbar \right) \approx 1 - \frac{i \Delta t}{\hbar} \hbar + \frac{1}{2!} \left( -\frac{i \Delta t}{\hbar} \right)^2 \hbar^2 + \cdots + \frac{1}{\nu_{\max}!} \left( -\frac{i \Delta t}{\hbar} \right)^{\nu_{\max}} \hbar^{\nu_{\max}}, \quad (3.9) \]
where \( \nu_{\max} \) is an integer number. In our calculations, we have used the fixed number \( \nu_{\max} = 10 \).

Since we use the harmonic oscillator wave functions as basis functions, the wave function \( \psi_j(r, t_n) \) and the one-body Hamiltonian \( \hbar \) are expressed as vectors and a matrix, respectively. The time integration in Eq. (3.7) is achieved by applying a series of matrix multiplication as in Eq. (3.9) to the vector representing the wave function \( \psi_j(r, t_n) \). The initial conditions \( \psi_j(r, 0) \) \((j = 1, \cdots, A')\) are taken to be the CHF solutions, which were obtained in the previous subsection. Starting the time integrations in Eq. (3.6) from an arbitrary point on the CHF line, we obtain a TDHF trajectory in the multi-dimensional TDHF manifold.

With the goal of studying the structural change of the TDHF trajectory starting from an arbitrary point on the CHF line, we apply the TR method discussed in § 2.3. In this method, we choose a set of representative points on the TDHF trajectory as the reference states. Taking a single-Slater determinant state described by the set of time-dependent single-particle wave functions \( \{ \psi_j(r, t); j = 1, \cdots, A' \} \) as the reference state \( |\phi_{\text{ref}}\rangle \), we carried out the iteration process from the step 1 to 4 discussed in § 2.3.
A Numerical Study on the Structure Change of Collective Motions

Here, it is to be noted that, though the reference state consists of complex wave functions, the vectors representing the wave functions $\phi(r)$ in the iterative process are taken to be real, since we are going to determine the wave functions satisfying the HF condition. The MOC plays an essential role also in this case in the iterative process of finding the self-consistent solutions. Typical numerical results are given in Figs. 10~12. In these figures, the TDHF trajectories in the multi-dimensional phase space are represented by the time dependence of the value of deformation calculated from the density in Eq. (3·5).

a) Ground state branch

Let us discuss the properties of the TDHF trajectories starting from an arbitrary point of the lowest CHF line, which passes through the lowest HF state. The time development of the trajectory is expressed in the deformation coordinate (collective subspace), which is shown in Fig. 10(a). As is clearly seen from this figure, the TDHF trajectories starting from the lowest CHF line are always oscillating around the ground state, irrespective of the initial amplitude. In this case, the TDHF trajectories display regular motion, and the lowest CHF line projected onto the collective

![Figure 10](https://academic.oup.com/ptp/article-abstract/95/5/883/1866518)

Fig. 10. (a) Density oscillations with small (full curve) and large (dashed curve) excitation energies. The resulting points obtained by the TR method are shown by open rhombuses (small amplitude) and pluses (larger amplitude). These are identical to the ground state. The iteration processes (dashed curves) of the TR method are shown for small-amplitude (b) and larger-amplitude (c) TDHF trajectories. The parabola represents the ground state branch in Fig. 9. The open rhombuses on the parabola in (b) and (c) denote the calculated points in the local configuration dictated (LCD) method.
subspace may be regarded as the collective PES which characterizes the TDHF trajectories. This statement is also consistent with the numerical results obtained by the TR method, also illustrated in Fig. 10. In Figs. 10(b) and (c), the convergence process of the TR method started from various representative points on the TDHF trajectory is shown for the two cases with the small- and the large-amplitude initial conditions. In the small-amplitude case, shown in Fig. 10(b), the first iteration already produces a state very near to the CHF line, and every solution of the TR method converges to the HF ground state, no matter where the initial reference state is located on the TDHF trajectory. In the large-amplitude case, which is depicted in Fig. 10(c), some solutions are eventually kicked out to the higher energy region during the iteration processes. This is caused by the fact that the wave function considered in our iteration process in the TR method is chosen so that the MOC is satisfied. In spite of the large fluctuations, the iteration processes always lead to the HF ground state. These cases in Fig. 10 correspond to Figs. 6 and 7 in the SU(3) model case in § 2.

b) Branch from high-lying state “2”

The numerical results for the TDHF trajectories starting from the arbitrary points on the high lying CHF line, which passes through the high-lying HF state labelled as “2” in Fig. 9, are shown in Figs. 11 and 12.

When the amplitude of the TDHF trajectory is small, as illustrated in Fig. 11(a), the TDHF trajectory mapped onto the collective subspace oscillates in the neighborhood of the high-lying HF state “2”. Though the behavior of the oscillation is not as simple as that of the small amplitude motion around the HF ground state, the
destination obtained by the TR method is only one, i.e., the high-lying HF state "2". The convergence process of the TR method is shown in Fig. 11(b). This case also corresponds to Figs. 6 and 7 in the $SU(3)$ model case in § 2.

When the relative excitation energy becomes higher, as shown in Fig. 12(a), the TDHF trajectory expressed in the collective subspace displays rather irregular large-amplitude oscillation. To study the properties of this irregular motion, we apply the TR method to the TDHF trajectory, whose iteration process is depicted in Fig. 12(b). As is clearly seen from Figs. 12(a) and (b), we can find three different local minimum points. One of these is the high-lying HF state "2", which is found in the small amplitude motion. The other two minimum points are detected when the excitation energy becomes high. These two minima are lower in energy than the high-lying HF state "2". This situation corresponds to the case of the $SU(3)$ model illustrated in Fig. 8, where the TDHF trajectory is characterized by multiple minimum points. From Figs. 11 and 12, we can easily imagine the geometrical structure around the high-lying HF state. It is located at the bottom of a small well and is accompanied by two different minimum points with lower energies.

§ 4. Summary and discussions

Making use of a simple model Hamiltonian, we have discussed the relation between the TDHF trajectories and the CHF lines in the TDHF coordinate space. Since we are interested in the collective motion, we have concentrated our discussion on the collective TDHF trajectories, which start from an arbitrary point on the CHF lines. When one projects the CHF lines onto the collective subspace, which is characterized by the constraining operator through the relation $(2 \cdot 12)$, one is involved in the question of whether the adiabatic collective PES or continuous collective PES
is appropriate for describing the collective motion. It turns out that the small-amplitude oscillation around the local HF state is well characterized by the continuous collective potential, which is the projection of the CHF line passing through the HF state under discussion onto the collective subspace. This situation remains unchanged, as long as the collective trajectory is connected with only one HF point. By calculating the collective TDHF trajectories, it was shown that the structural change of the collective motion occurs when the number of local minima connected with the trajectory changes. In this case, one has to introduce additional degrees of freedom to describe the structural change of the collective motion, by properly identifying the existence of more than one local minimum although the collective motion seems to be controlled by the adiabatic collective PES. By applying the new numerical method to a more realistic case, it was shown that the proposed method is feasible for a more complicated system.

Since the HF states thus obtained for describing the structural change of collective motion may be well characterized by the difference of the configuration among them, one may easily find an additional degree of freedom, which should be treated explicitly, in addition to the collective coordinates. By applying the self-consistent collective coordinate method, in the separate paper, it is discussed how to explicitly include the new degrees of freedom in the band-crossing region, where more than two CHF lines come close to each other. By combining these two approaches, one may clarify the proper meaning of the adiabatic and diabatic single-particle orbitals, as well as the adiabatic and diabatic collective PES in the actual situation appearing in Fig. 1, which will be reported in a subsequent paper.

References