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Physical review C

Volume 50, Number 1, Page 138-147, 1994

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doi: 10.1103/PhysRevC.50.138
Nonlinear resonance in the time-dependent Hartree-Fock manifold

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(Received 17 August 1993; revised manuscript received 11 March 1994)

In order to try to open a new scope to explore the mutual dependence between the single-particle and collective modes of motion near to the level crossing region, a general method is developed to investigate the nonlinear resonant structure of the time-dependent Hartree-Fock (TDHF) manifold, without depending on the adiabatic assumption. By using the Lie canonical transformation with the Depri perturbation treatment, in this method, the maximal integrable-form representation of the TDHF manifold is introduced. This representation plays an essential role in exploring the nonlinear resonant structure of the TDHF manifold, which characterizes complex topology of the manifold. Aiming at relating the nonlinear resonance in the TDHF manifold with the dynamics between the single-particle and collective modes of motion near to the level crossing region, structure of the TDHF wave function is investigated. It is clarified that an isolated nonlinear resonant region of the TDHF manifold is characterized by a local constant of motion (dynamical symmetry) and generates a new type of dynamical stable single-Slater-determinant states, which is topologically different from the TDHF states near the HF ground state, and cannot be reached by the conventional static Hartree-Fock method, constrained Hartree-Fock method, nor the adiabatic TDHF theories. One may expect that the appearance mechanism of the new dynamical stable single-Slater-determinant states gives us a new scope for understanding occurrence mechanism of a variety of collective sideband structure near to the level crossing region.

PACS number(s): 21.60 Ev, 21.60 Jz, 21.10 Re

I. INTRODUCTION

It has been the central theme in the microscopic theory of nuclear collective dynamics to develop a method that is capable of describing various states situated far from a certain stable mean-field, a dynamical interrelationship among many stable mean fields with different symmetries, the “phase transition” in the finite many-fermion system as the nucleus, etc.

In the development of the nuclear structure physics, the importance of the mutual dependence between the single-particle and collective degrees of freedom in the level crossing region has been discussed repeatedly [1–10]. These statements have been mainly drawn from the adiabatic time-dependent perturbation theory like the adiabatic time-dependent Hartree-Fock (ATDHF) [11–15] theory, which is usually grounded upon the constrained Hartree-Fock (CHF) or configuration-CHF theories. Since the adiabatic assumption does not hold near the level crossing region, it is imperative to carefully figure out the mutual dynamics between the single-particle and collective degrees of freedom, by going beyond the adiabatic (or diabatic) assumption.

The TDHF equation is formally expressed as the canonical equations of motion in the classical mechanics [16–19], when a set of time-dependent parameters specifying the TDHF single-Slater-determinant state is suitably chosen. The parameter space is called a TDHF (symplectic) manifold. A relation between the TDHF trajectories in the TDHF-manifold and the full quantum excited states has been one of the main theoretical issues in developing the theory of large-amplitude collective motion [18,20,21]. Another important issue is how to understand the complex structure of the TDHF manifold, which is supposed to contain relevant semiclassical information on the dynamical property of large-amplitude collective motion in the level crossing region. In this paper, we treat the latter problem. By exploiting the symplectic structure of the TDHF manifold and by applying the general theory of nonlinear dynamical system [22–24], we try to formulate the nonlinear dynamical mean-field theory for the finite, quantum many-fermion systems of the nucleus, and try to open a new way of exploring the dynamics between the single-particle and collective modes of motion near the level crossing region without depending on the adiabatic assumption.

One of the cornerstones in developing the classical dynamical theory has been making clear why the phase space shows an inexhaustibly rich structure even in a simple classical system with only two degrees of freedom. In these studies, it has turned out to be decisive to obtain analytic information on each fixed point, including nonlinear resonant point. It may not be an exaggeration to say that the history of the nonlinear dynamics has been a struggle to develop the proper perturbation theory for obtaining the (approximate) invariant, which provides us with analytic information on the nonlinear resonant structure of the phase space. In Secs. II and III, we discuss how to obtain the approximate invariants (approximate constants of motion) of the TDHF manifold.
by using the Lie transformation method \[25,26\]. In order to get the Lie generating function, one usually employs the Deprit perturbation treatment \[27\] which is briefly summarized in Sec. II A.

By using the Lie transformations, in Sec. III, we discuss how to define a maximal integrable form representation where the approximate invariants manifest themselves explicitly. With the use of this representation, Secs. IV and V are devoted to investigating the nonlinear resonant structure of the TDHF-manifold and to discuss how it reflects on the single-particle and collective modes of motion. It is demonstrated that the nonlinear resonant structure of the TDHF manifold gives a local constant of motion, and leads us to a new type of stable single-Slater-determinant states which is topologically different from the TDHF states near the HF ground state and are not reached by the usual Hartree-Fock (HF), constrained Hartree (CHF) or ATDHF theories.

II. TDHF SYMPLECTIC MANIFOLD

A. Canonical-variable representation of the TDHF theory

A stationary stable mean-field is specified by a Hartree-Fock (HF) state of an \( N \)-nucleon system satisfying the variational principle

\[
\delta \langle \phi_0 | H | \phi_0 \rangle = 0. 
\] (2.1)

By using the single-nucleon operators \( \hat{c}_\alpha, \hat{c}_\alpha^\dagger \), \( | \phi_0 \rangle \) is expressed as

\[
| \phi_0 \rangle = \prod_{i=1}^N \hat{c}_i^\dagger | 0 \rangle, \quad \hat{c}_\alpha | 0 \rangle = 0. 
\] (2.2)

The single-nucleon states are then divided into the particle and hole states as

\[
\hat{c}_\alpha^\dagger = \begin{cases} 
\hat{a}_{\alpha, \mu}^\dagger, & \alpha > N, \quad \mu = N + 1, \ldots, N + M, \\
\hat{b}_i, & \alpha = N, \quad i = 1, \ldots, N,
\end{cases} 
\] (2.3)

where \( M \) denotes a number of particle states. The Hamiltonian in Eq. (2.1) is generally expressed as

\[
H = \sum_{\alpha} \varepsilon_\alpha : \hat{c}_\alpha^\dagger \hat{c}_\alpha : + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} V_{\alpha \beta, \gamma \delta} : \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \hat{c}_\gamma \hat{c}_\delta : , 
\] (2.4)

where the symbol : : represents the normal product with respect to the HF state \( | \phi_0 \rangle \).

A time-dependent mean field is specified by the general (time-dependent) single-Slater-determinant state \( | F \rangle \) as

\[
| F \rangle \equiv e^{\hat{F}} | \phi_0 \rangle, \quad \hat{F} \equiv \sum_{\mu i} (f_{\mu i} \hat{a}_{\mu i}^\dagger - f_{\mu i}^* \hat{b}_i), 
\] (2.5)

which covers the whole space of states of the \( N \)-fermion system. The basic equation to determine the time-dependence of the parameters \( f_{\mu i}, f_{\mu i}^* \) in \( | F \rangle \) is given by the TDHF equation\(^1\)

\[
\delta \langle F | i \frac{d}{dt} - \hat{H} | F \rangle = 0, 
\] (2.6)

which is known to be equivalent to the following canonical equations of motion;

\[
i \dot{C}_{\mu i} = \frac{\partial H}{\partial C_{\mu i}^*}, \quad i \dot{C}_{\mu i}^* = -\frac{\partial H}{\partial C_{\mu i}}, \quad H(C, C^*) \equiv \langle F | \hat{H} | F \rangle. 
\] (2.7)

Here a new set of canonical variables is introduced through the following variable transformation;

\[
C_{\mu i} = \left( \frac{\sin \sqrt{\int f^\dagger f} f^\dagger}{\sqrt{\int f^\dagger f}} \right)_{\mu i}, \quad C_{\mu i}^* = C_{\mu i}^\dagger = \left( \frac{\sin \sqrt{\int f f^\dagger}}{\sqrt{\int f f^\dagger}} \right)_{\mu i}. 
\] (2.8)

Equation (2.7) describes the TDHF trajectory and exhibits a symplectic structure of the TDHF manifold \[12-15\].

The quadratic part of the Hamiltonian in the \( (C, C^*) \) representation can be transformed to a normal form by a linear canonical transformation determined by the RPA:

\[
C_{\mu i} \equiv \eta_k, \quad k = 1, \ldots, K, \quad K = M \times N. 
\] (2.9)

After applying the canonical transformation in Eq. (2.9) to Eq. (2.7), one gets

\[
i \dot{\eta}_k = \frac{\partial \mathcal{H}}{\partial \eta_k^*}, \quad i \dot{\eta}_k^* = -\frac{\partial \mathcal{H}}{\partial \eta_k}, 
\] (2.10)

where

\[
\mathcal{H} = H(C(\eta, \eta^*), C^*(\eta, \eta^*)) = \mathcal{H}_0 + \varepsilon \mathcal{H}_1 + \varepsilon^2 \mathcal{H}_2 + \cdots + \sum_{n=\eta} \varepsilon^n \mathcal{H}_n , 
\]

\[
\mathcal{H}_0 = \sum_k \Omega_k \eta_k \eta_k^*, 
\]

\[
\mathcal{H}_1 = \sum_{k l m} \{(V_{k l m} \eta_k^* \eta_l^* \eta_m^* + V_{k l}^* \eta_k^* \eta_l^* \eta_m) + \text{c.c.}\}, 
\]

\[
\mathcal{H}_2 = \sum_{k l m} \{(V_{k l m} \eta_k^* \eta_l^* \eta_m^* \eta_m^* + V_{k l m}^* \eta_k^* \eta_l^* \eta_m \eta_m^*) \\
+ \frac{1}{2} V_{k l m} \eta_k^* \eta_l^* \eta_m \eta_m^*) + \text{c.c.}\}, 
\]

\[
\cdots, 
\]

(2.11)

here the interaction parameters \( V_{k l m} \) are related to the original ones \( V_{\alpha \beta, \gamma \delta} \) in Eq. (2.4) through Eqs. (2.8) and (2.9). In Eq. (2.11), \( \Omega_k \)'s stand for the RPA eigenfrequencies and an integer \( n + 1 \) in \( \mathcal{H}_n \) denotes a power of the normal-variables \( (\eta_k, \eta_k^*) \) contained in each term; \( \varepsilon \) expresses a real smallness parameter.

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\(^1\)In this paper, we use a convention \( \hbar = 1 \).
B. Lie canonical transformation

Let us start with summarizing the Lie canonical transformation theory [19,20] and introduce various notations used in the subsequent sections. Suppose we have a Lie generating function $W(X, \varepsilon)$ satisfying

$$\frac{dX_\lambda}{d\varepsilon} = \{X_\lambda, W(X, \varepsilon)\}_{PB},$$

(2.12)

where the symbol $\{ \cdots \}$ means the Poisson bracket with respect to variables $(X_\lambda, X_\lambda^*)$ defined by

$$\{A, B\}_{PB} \equiv \sum_\lambda \left\{ \frac{\partial A}{\partial X_\lambda} \frac{\partial B}{\partial X_\lambda^*} - \frac{\partial A}{\partial X_\lambda^*} \frac{\partial B}{\partial X_\lambda} \right\}.$$  

(2.13)

Equation (2.12) is reduced to a set of canonical equations of motion when one regards $\varepsilon$ as the “time” and $-iW$ as the “Hamiltonian.” Namely, the solution of Eq. (2.12) expressed as

$$X_\lambda = X_\lambda(X^{(0)}, \varepsilon),$$

(2.14)

with the initial condition

$$X_\lambda(X^{(0)}, \varepsilon = 0) = X^{(0)}_\lambda,$$

(2.15)

describes a canonical transformation $(X^{(0)}, X^{\ast(0)}) \leftrightarrow (X, X^*)$. An evolution operator $T$ representing the above canonical transformation is introduced as follows: A function $f(X^{(0)})$ of the initial coordinates is derived from a function $g(X)$ of the transformed coordinates by operating $T$ onto $g(X^{(0)})$ as

$$f(X^{(0)}) = Tg(X^{(0)}) = g(X(X^{(0)}, \varepsilon)).$$

(2.16)

If $g$ is identity, one has a relation

$$X_\lambda = TX^{(0)}_\lambda.$$  

(2.17)

Substituting Eq. (2.17) for Eq. (2.12), one gets

$$\frac{dT}{d\varepsilon} X^{(0)}_\lambda = T\{X^{(0)}_\lambda, W(X^{(0)}, \varepsilon)\}_{PB}. $$

(2.18)

Introducing a Lie operator defined by

$$L(\varepsilon) \equiv \{W(X^{(0)}, \varepsilon), \ast\}_{PB},$$

(2.19)

one obtains

$$\frac{dT}{d\varepsilon} X^{(0)}_\lambda = -TL(\varepsilon)X^{(0)}_\lambda, \quad \text{i.e.} \quad \frac{dT}{d\varepsilon} = -TL(\varepsilon),$$

(2.20)

whose formal solution is expressed as

$$T = \exp \left( -\int^\varepsilon L(\varepsilon') d\varepsilon' \right).$$

(2.21)

Now, let us apply the Lie canonical transformation to the Hamiltonian (2.11) whose variables $(\eta, \eta^*)$ are regarded to be the initial variables $(X^{(0)}, X^{\ast(0)})$. With the use of Eq. (2.16) (with correspondence $f \leftrightarrow \mathcal{H}$ and $g \leftrightarrow \mathcal{H}$), the transformed Hamiltonian $\mathcal{H}(X)$ is then written as

$$\mathcal{H}(X(X^{(0)}, \varepsilon)) = \mathcal{H}(X^{(0)}),$$

(2.22a)

which is expressed as

$$T\mathcal{H}(X^{(0)}) = \mathcal{H}(X^{(0)}), \quad \text{i.e.} \quad \mathcal{H}(X^{(0)}) = T^{-1}\mathcal{H}(X^{(0)}).$$

(2.22b)

By changing the arguments, one finally gets

$$\mathcal{H}(X) = T^{-1}\mathcal{H}(X).$$

(2.23)

The evolution operator $T$ is usually obtained perturbatively by using a method proposed by Deprit [27]. In this method, every quantity is assumed to be an analytic function of $\varepsilon$. In the same way as the Hamiltonian in Eq. (2.11), one may thus introduce the following expansion form:

$$\mathcal{H} = \sum_{n=0}^{\infty} \varepsilon^n \mathcal{H}_n, \quad T = \sum_{n=0}^{\infty} \varepsilon^n T_n, \quad W = \sum_{n=0}^{\infty} \varepsilon^n W_{n+1},$$

$$L = \sum_{n=0}^{\infty} \varepsilon^n L_{n+1}, \quad L_{n+1} \equiv \{W_{n+1}, \ast\}_{PB}. $$

(2.24)

Substituting Eq. (2.24) for Eq. (2.20), one gets

$$T_n = -\frac{1}{n} \sum_{m=0}^{n-1} T_m L_{n-m}.$$  

(2.25)

The initial condition for the evolution operator $T$ is derived from the condition (2.15) and is given by

$$T_0 = 1.$$  

(2.26)

With the aid of Eq.(2.26), the set of successive relations in Eq. (2.25) is expressed as

$$T_1 = -L_1, \quad T_2 = -\frac{1}{3} L_2 + \frac{1}{3} L_3^2,$$

$$T_3 = -\frac{1}{3} L_3 + \frac{1}{3} L_2 L_1 + \frac{1}{3} L_2 L_1 + \frac{1}{6} L_3 L_1,$$

(2.27)

For the inverse operator $T^{-1}$ satisfying $T^{-1}T = 1$, one has

$$T_1^{-1} = L_1, \quad T_2^{-1} = \frac{1}{3} L_2 + \frac{1}{3} L_3^2,$$

$$T_3^{-1} = \frac{1}{3} L_3 + \frac{1}{3} L_2 L_1 + \frac{1}{3} L_2 L_1 + \frac{1}{6} L_3 L_1,$$

(2.28)

where the condition $T_0^{-1} = 1$ compatible with Eq.(2.26) has been used. The explicit form of the transformed Hamiltonian is then given as

$$\mathcal{H}_0 = T_0^{-1}\mathcal{H}_0 = \mathcal{H}_0,$$

(2.29a)

$$\mathcal{H}_1 = T_0^{-1}\mathcal{H}_1 + T_0^{-1}\mathcal{H}_0 = \mathcal{H}_1 + \{W_1, \mathcal{H}_0\}_{PB},$$

(2.29b)

$$\mathcal{H}_2 = T_0^{-1}\mathcal{H}_2 + T_1^{-1}\mathcal{H}_1 + T_0^{-1}\mathcal{H}_0,$$

$$= \mathcal{H}_2 + \{W_1, \mathcal{H}_1\}_{PB} + \frac{1}{2} \{W_1, \{W_1, \mathcal{H}_0\}_{PB}}$$

(2.29c)

The above discussion is quite general and the generating function $W$ is still left unspecified. In what follows, we will discuss how to define the generating function $W$ by requiring that the transformed Hamiltonian is of the maximal integrable form.
III. MAXIMAL INTEGRABLE-FORM REPRESENTATION

A. Integrable form of Hamiltonian

In a region near to a certain stationary stable point in the TDHF manifold (corresponding to the HF stationary state), the small amplitude oscillation is well described by the harmonic approximation (RPA). The Hamiltonian of the harmonic oscillators is expressed by action variables alone, when an action-angle representation is adopted instead of the conventional coordinate and momentum variables. This means that the harmonic motions are integrable and the actions are nothing but the constants of motion. When there exist nonlinear interactions, the system is no longer integrable and the action variables are not constants of motion any more. According to the KAM theorem [28], however, the action variables still remain approximate invariant in the vicinity of the stable point, provided the KAM condition holds. It is then very important to study how an approximate invariant transfigures under the effects of nonlinear interaction.

This problem has a special relevance to the nuclear collective dynamics, because it is one of the most important questions in exploring what kinds of dynamical change will take place on the collective mode when the noncollective modes of motion are excited. A well-known example is the various sideband structure of the collective motion in the level crossing region.

To investigate this problem, it is convenient to introduce the action-angle representation through

$$\tilde{\eta}_k \equiv \sqrt{J_k} \exp(-i\phi_k).$$

When the Hamiltonian in Eq. (2.11) is expressed by the action variables ($J_k$) alone, one may easily find the constants of motion. When the Hamiltonian has an explicit angle-variable dependence, it is of vital importance to introduce the maximal integrable-form representation where the angle dependence of the Hamiltonian is optimally eliminated by using the nonlinear canonical transformation discussed in Sec. II B given by

$$\tilde{\eta}_k = T\eta_k \left[ \tilde{\eta}_k \equiv \sqrt{J_k} \exp(-i\phi_k) \right].$$

To demonstrate how to introduce the maximal integrable-form representation, let us start with considering a simplified case where the RPA frequencies $\Omega_k$ are nonresonant. Since the nonlinear effects is assumed to be sufficiently small near the HF state, it is reasonable to apply the Druperturbation method. In the following, we discuss how the maximal integrable-form representation plays an essential role in studying transfiguration of an approximate invariant and in studying an applicability of the Druperturbation method, as one goes away from the HF state. In the nonresonant case, the canonical transformation to the maximal integrable-form representation is determined in such a way that the resultant Hamiltonian is written by a new set of action variables alone, i.e.

$$\mathcal{H}(\tilde{\eta}^*, \tilde{\eta}) = T^{-1} \mathcal{H}(\tilde{\eta}^*, \tilde{\eta}) = \mathcal{H}(\tilde{J}), \quad \tilde{J}_k \equiv \tilde{\eta}_k^* \tilde{\eta}_k. \quad (3.3)$$

The Lie generating function, which transforms the Hamiltonian into the integrable form, is obtained in the following way. In accordance with the initial condition for the evolution operator in Eq. (2.26), the lowest-order Hamiltonian is given by

$$\mathcal{H}_0 = \sum_k \Omega_k \tilde{J}_k. \quad (3.4)$$

The first-order Hamiltonian $\mathcal{H}_1$ appearing in Eq. (2.29b) is a cubic function of $(\tilde{\eta}, \tilde{\eta}^*)$ by definition, and is expressed as

$$\mathcal{H}_1 = \sum_{klm} \left\{ \left( V_{klm} \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* + V_{klm}^n \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* \right) + c.c. \right\} + \{ W_1, \mathcal{H}_0 \}_{PB}, \quad (3.5)$$

where the unknown function $W_1$ is assumed to have the following general cubic form;

$$W_1 = \sum^{kilm} \left\{ \left( W_{klm} \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* + W_{klm}^n \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* \right) - c.c. \right\}. \quad (3.6)$$

The explicit form of the second term in the rhs of Eq. (3.5) is given by

$$\{ W_1, \mathcal{H}_0 \}_{PB} = \sum_k \Omega_k \left( \frac{\partial}{\partial \tilde{\eta}_k} - \frac{\partial}{\partial \tilde{\eta}_k^*} \right) W_1,$n

$$= \sum^{kilm} \{ -(\Omega_k + \Omega_l + \Omega_m) W_{klm} \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* - (\Omega_k + \Omega_l - \Omega_m) W_{klm}^n \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* \} + c.c. \}. \quad (3.7)$$

The unknown coefficients $W_{klm}$ and $W_{klm}^n$ in $W_1$ are determined by requiring that the first-order resultant Hamiltonian has no angle dependence, i.e., $\mathcal{H}_1 = 0$. The coefficients determined under this requirement are

$$W_{klm} = V_{klm} (\Omega_k + \Omega_l + \Omega_m)^{-1}, \quad W_{klm}^n = V_{klm}^n (\Omega_k + \Omega_l - \Omega_m)^{-1}. \quad (3.8)$$

The second-order Hamiltonian $\mathcal{H}_2$ in Eq. (2.29c) is expressed as

$$\mathcal{H}_2 = \sum^{kilmn} \left\{ \left( V_{klmn} \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* \tilde{\eta}_n^* + V_{klmn} \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* \tilde{\eta}_n^* + \frac{1}{2} V_{klmn}^n \tilde{\eta}_k^* \tilde{\eta}_l^* \tilde{\eta}_m^* \tilde{\eta}_n^* \right) + c.c. \right\} + \frac{1}{2} \{ W_1, \mathcal{H}_1 \}_{PB} + \frac{1}{2} \{ W_2, \mathcal{H}_0 \}_{PB}, \quad (3.9)$$
where the following relation has been used;

\[ \mathcal{H}_1 = -\{W_1, \mathcal{H}_0\}_{PB}. \]  

(3.10)

In the same way as in Eq. (3.6), the unknown second-order Lie generating function \( W_2 \) is assumed to have the general form given by

\[ W_2 = \sum_{klmn} \{(W_{klmn} \bar{\eta}_k \bar{\eta}_l \bar{\eta}_m \bar{\eta}_n + W_{klmn}^{n} \bar{\eta}_k \bar{\eta}_l \bar{\eta}_m \bar{\eta}_n + W_{klmn}^{mn} \bar{\eta}_k \bar{\eta}_l \bar{\eta}_m \bar{\eta}_n) - \text{c.c.}\}. \]  

(3.11)

By using Eq. (3.11), the third term in the rhs of Eq. (3.9) is expressed as

\[ \{W_2, \mathcal{H}_0\}_{PB} = \sum_{i} \Omega_i \left( \bar{\eta}_i \frac{\partial}{\partial \bar{\eta}_i} - \bar{\eta}^*_i \frac{\partial}{\partial \bar{\eta}^*_i} \right) W_2 \]

\[ = \sum_{klmn} \{-\Omega_k + \Omega_l + \Omega_m + \Omega_n\} \{W_{klmn} \bar{\eta}_k \bar{\eta}_l \bar{\eta}_m \bar{\eta}_n - (\Omega_k + \Omega_l + \Omega_m - \Omega_n) \}

\[ - (\Omega_k + \Omega_l - \Omega_m - \Omega_n) \} \]  

(3.12)

Using the known quantity \( W_1 \), the second term in the rhs of Eq. (3.9) is expressed as

\[ \{W_1, \mathcal{H}_1\}_{PB} = \sum_{klmnt} \{(3W_{kl}^{i} V_{mnt} - 3W_{kl}^{n} V_{mn}^{i}) \bar{\eta}_k \bar{\eta}_l \bar{\eta}_m \bar{\eta}_n \]

\[ + (2W_{kl}^{i} V_{mnt} - 6W_{kl}^{n} V_{mnt} - 6W_{kl}^{n} V_{mnt} - 2W_{kl}^{n} V_{mnt}) \bar{\eta}_k \bar{\eta}_l \bar{\eta}_m \bar{\eta}_n \]

\[ + (W_{kl}^{i} V_{mnt} - 9W_{kl}^{n} V_{mnt} - 4W_{kl}^{n} V_{mnt}) \bar{\eta}_k \bar{\eta}_l \bar{\eta}_m \bar{\eta}_n + \text{c.c.}\}. \]  

(3.13)

By requiring the elimination of the angle dependence of the second-order Hamiltonian, the unknown coefficients in \( W_2 \) are determined as

\[ W_{klmn} = \left\{ 2V_{klmn} + 3 \sum (W_{kl}^{i} V_{mnt} - W_{kl}^{n} V_{mn}^{i}) \right\} (\Omega_k + \Omega_l + \Omega_m + \Omega_n)^{-1}, \]

\[ W_{kl}^{n} = \left\{ 2V_{kl}^{n} + 2 \sum (W_{kl}^{i} V_{mnt} - 3W_{kl}^{n} V_{mnt} - 3W_{kl}^{n} V_{mnt} - W_{kl}^{n} V_{mnt}) \right\} (\Omega_k + \Omega_l + \Omega_m - \Omega_n)^{-1}, \]

\[ W_{kl}^{mn} = \left\{ V_{kl}^{mn} + \sum (W_{kl}^{i} V_{mnt} - 9W_{kl}^{n} V_{mnt} - 4W_{kl}^{n} V_{mnt}) \right\} (\Omega_k + \Omega_l - \Omega_m - \Omega_n)^{-1}, \]

\[ W_{kl} = W_{lk} = 0. \]  

(3.14)

The resultant second-order Hamiltonian is then expressed as

\[ \mathcal{H}_2 = \sum_{kl} \left\{ V_{kl}^{i} + \frac{1}{2} \sum (W_{kl}^{i} V_{kl}^{*} - 9W_{kl}^{n} V_{kl}^{i} - 4W_{kl}^{n} V_{kl}^{i} + \text{c.c.}) \right\} J_k \dot{J}_l, \]

\[ + V_{kl}^{i} + \frac{1}{2} \sum (W_{kl}^{i} V_{kl}^{*} - 9W_{kl}^{n} V_{kl}^{i} - 4W_{kl}^{n} V_{kl}^{i} + \text{c.c.}) \dot{J}_k \dot{J}_l, \]  

(3.15)

which contains only the new action variables \( \dot{J}_k \).

In this way, one may determine the Lie generating functions as well as the transformed Hamiltonian up to the desired order. The resultant Hamiltonian \( \mathcal{H} \) is expressed by only the new action variables

\[ J_k = \bar{\eta}_k \dot{\eta}_k = T J_k = J_k + \{W_1, J_k\}_{PB} + \cdots, \]  

(3.16)

which just correspond to the constants of motion.

B. Maximal integrable-form representation

In the previous subsection, we have discussed the method of obtaining the regular trajectories within the framework of the Lie transformation with Deprit perturbation method. Generally, one may encounter the resonant cases among the RPA eigenfrequencies. In such cases, the above perturbation method has the well-known difficulty of small denominator problem: If there hold resonant conditions among the RPA eigenfrequencies,

\[ m \Omega_k - n \Omega_l = 0, \]

(3.17)

one cannot eliminate the corresponding angle-dependent
terms of the Hamiltonian, which is clearly seen from Eqs. (3.8) and (3.14). Thus, the transformed Hamiltonian after the Lie transformation given in the previous subsection has the following form [29]:

\[ \mathcal{H} = \mathcal{H}_{\text{integ}}(\tilde{J}_1, \ldots, \tilde{J}_K) + \mathcal{H}_{\text{coul}}(\tilde{J}_1, \ldots, \tilde{J}_K; \tilde{\phi}_1, \ldots, \tilde{\phi}_K), \]  

(3.18)

where \( \mathcal{H}_{\text{integ}} \) stands for the integrable part described by the new action variables \( \tilde{J}_K \) alone, and \( \mathcal{H}_{\text{coul}} \) means the coupling terms which cannot be eliminated due to the resonant condition such as Eq. (3.17). In this way, the maximal integrable-form representation is defined as the most natural canonical coordinate system [22] in the TDHF-manifold, where the major terms in the Hamiltonian are incorporated into the integrable part of the transformed Hamiltonian as much as possible, by only leaving the coupling terms which cannot be eliminated by the Deprit perturbation treatment based on the HF state \( |\phi_0\rangle \).

Here it must be noticed that the maximal integrable-form representation is a local concept, which is specific for the stable HF state \( |\phi_0\rangle \). If one wants to study the structure of the TDHF manifold in the vicinity of another HF state \( |\phi'_0\rangle \), it is natural to start with another canonical coordinate system \( (C', C'^*) \) instead of \( (C, C^*) \) in Eq. (2.8) and introduce a maximal integrable-form representation specific for the new HF state \( |\phi'_0\rangle \).

IV. NONLINEAR RESONANCE AND ASSOCIATED CONSTANTS OF MOTION

A. Elliptic and hyperbolic fixed points

At the end of the previous section, it has been clarified that the maximal integrable-form representation is of vital importance in discussing the nonlinear resonant structure of the TDHF manifold in an analytical way. In this section, we discuss how the nonlinear resonance appearing in the TDHF manifold is elucidated by means of the maximal integrable-form representation.

To make the discussion simple, we consider the following system with two degrees of freedom. A pair of coordinates \((\eta_1, \eta_2)\) is supposed to describe the collective motion under consideration and the other pair of coordinates \((\eta_2, \eta'_2)\) describes the noncollective motion in the maximal integrable-form representation. In this representation, the Hamiltonian is expressed as

\[ \mathcal{H} = \mathcal{H}_{\text{integ}}(\tilde{J}_1, \tilde{J}_2) + \mathcal{H}_{\text{coul}}(\tilde{J}_1, \tilde{J}_2; \tilde{\phi}_1, \tilde{\phi}_2), \]  

(4.1)

where

\[ \tilde{\eta}_1 = \sqrt{J_1}e^{-i\tilde{\phi}_1}, \quad \tilde{\eta}_2 = \sqrt{J_2}e^{-i\tilde{\phi}_2}. \]  

(4.2)

The nonlinear resonant condition is determined by the integrable part of the Hamiltonian \( \mathcal{H}_{\text{integ}}(\tilde{J}_1, \tilde{J}_2) \), and is given by

\[ r\omega_1(\tilde{J}_1, \tilde{J}_2) - s\omega_2(\tilde{J}_1, \tilde{J}_2) = 0, \]

where \( r \) and \( s \) being a prime number, respectively, (4.3)

with

\[ \omega_1(\tilde{J}_1, \tilde{J}_2) = \frac{\partial \mathcal{H}_{\text{integ}}(\tilde{J}_1, \tilde{J}_2)}{\partial \tilde{J}_1}, \]

and

\[ \omega_2(\tilde{J}_1, \tilde{J}_2) = \frac{\partial \mathcal{H}_{\text{integ}}(\tilde{J}_1, \tilde{J}_2)}{\partial \tilde{J}_2}. \]

(4.4)

When the nonlinear resonance satisfying Eq. (4.3) occurs, the standard perturbation method is involved into the well-known difficulty of small denominator problem, treating such terms in the Fourier series of \( \mathcal{H}_{\text{coul}} \) that have angle-variable dependence \( n(r\tilde{\phi}_1 - s\tilde{\phi}_2) \) with \( n = 1, 2, \ldots \). For an isolated nonlinear resonance where the resonant point \( (\tilde{J}_1^{(0)}, \tilde{J}_2^{(0)}) \) satisfying Eq. (4.3) is sufficiently far from the other nonlinear resonances, the above secularity is eliminated in the following way, developed in the classical nonlinear dynamics [22].

Provided that we are interested in a region near to the resonant point \( (\tilde{J}_1^{(0)}, \tilde{J}_2^{(0)}) \), it is general enough to consider only the Fourier components of \( \mathcal{H}_{\text{coul}} \) such as

\[ \mathcal{H}_{\text{coul}}(\tilde{J}_1, \tilde{J}_2; \tilde{\phi}_1, \tilde{\phi}_2) \]

\[ \Rightarrow \sum_n V^{(n)}(\tilde{J}_1, \tilde{J}_2) \left\{ e^{in(r\tilde{\phi}_1 - s\tilde{\phi}_2)} + \text{c.c.} \right\}. \]  

(4.5)

Let us introduce the following canonical transformation \( (\tilde{J}, \tilde{\phi}) \leftrightarrow (I, \theta) \) whose generating function is given by

\[ W = -(r\tilde{\phi}_1 - s\tilde{\phi}_2)I_2 + \tilde{\phi}_1I_1. \]  

(4.6)

By means of \( W \), the old canonical variables are expressed by the new ones as

\[ \tilde{\phi}_1 = \theta_1, \quad \tilde{\phi}_2 = \frac{1}{s}(\theta_2 + r\theta_1), \quad \tilde{I}_1 = I_1 - rI_2, \quad \tilde{I}_2 = sI_2. \]  

(4.7)

Substituting Eq. (4.7) into Eqs. (4.1) and (4.5), one gets a new Hamiltonian \( \mathcal{H} \) given by

\[ \mathcal{H} = \mathcal{H}_{\text{integ}} + \mathcal{H}_{\text{coul}}, \]

\[ \mathcal{H}_{\text{integ}} = \mathcal{H}_{\text{integ}}(\tilde{J}(I)), \]

\[ \mathcal{H}_{\text{coul}} = \mathcal{H}_{\text{coul}}(\tilde{J}(I)\phi(\theta)) \]

\[ = \sum_n 2V^{(n)}(\tilde{J}(I))\cos(n\theta). \]  

(4.8)

As is clearly seen from Eq. (4.8), the new Hamiltonian \( \mathcal{H} \) does not depend on \( \theta_1 \), indicating an existence of a new local constant of motion \( I_1 \). Consequently the system described by the Hamiltonian in Eq. (4.8) is effectively reduced into a system with one degree of freedom \( (I_2, \theta_2) \) which is integrable.

An important conclusion from the above discussion is summarized as follows: By employing the maximal integrable-form representation referred to the stable HF state \( |\phi_0\rangle \), it has been clarified that an appearance of an isolated resonance indicates an existence of both a new local constant of motion \( I_1 \) and a new local regular mo-
tion [described by \((I_2, \theta_2)\)] in the vicinity of the resonant point. The variables \((I_1, \theta_1)\) are regarded as describing a transfigured collective motion and the variables \((I_2, \theta_2)\) are supposed to describe transfigured noncollective motion in the nonlinear resonant region. With the aid of Eq. (4.8), one may get a set of elliptic (stable) and hyperbolic (unstable) fixed points \((I_2^{(0)}, \theta_2^{(0)})\) in the \(I_2-\theta_2\) phase plane at

\[
\frac{\partial H}{\partial \theta_2}
|_{(I_2^{(0)}, \theta_2^{(0)})} = \frac{\partial H}{\partial I_2}
|_{(I_2^{(0)}, \theta_2^{(0)})} = 0,
\]

for a given value \(I_1\) in the nonlinear resonant region.

**B. Illustrative example**

In order to illustrate a feasibility of the method proposed in the present and previous sections, let us consider the following SU(3) Hamiltonian given by

\[
\hat{H} = \sum_{i=0}^{2} \varepsilon_i \hat{K}_{ii} + \frac{V}{2} \sum_{i=1}^{2} (\hat{K}_{ii} \hat{K}_{ii} + H.c.),
\]

\[
\hat{K}_{ij} = \sum_{m=1}^{N} \hat{c}_{im}^\dagger \hat{c}_{jm},
\]

There are three orbits with energies \(\varepsilon_0 < \varepsilon_1 < \varepsilon_2\) and each level has \(N\)-fold degeneracy. In the following calculation, we treat a system with even particle number \(N\). With the aid of canonical variables in Eq. (2.8), the Hamiltonian in the TDHF-manifold is expressed as

\[
H(C, C^*) = \varepsilon_0 N + (\varepsilon_1 - \varepsilon_0)C_1^*C_1 + (\varepsilon_2 - \varepsilon_0)C_2^*C_2
+ V(N-1)(C_1^2 + C_2^2 + C_1^2 + C_2^2)
\times (N - C_1^*C_1 - C_2^*C_2).
\]

The used parameters are \(N = 30, \varepsilon_0 = 0, \varepsilon_1 = 1, \varepsilon_2 = 2\), and \(V = -0.01\). By introducing the coordinates and momenta through

\[
q_j = (C_j^* + C_j)/\sqrt{2}, \quad p_j = i(C_j^* - C_j)/\sqrt{2},
\]

the Poincaré section of the TDHF trajectories on a plane \((p_1, q_1)\) is constructed with a condition \(q_2 = 0\). In the present case with weak interaction, the Poincaré sections with various total energies usually indicate regular motion expressed by concentric circles centered at the origin. As the system gets more energy, the structure of the TDHF manifold is affected by the nonlinear interaction. The Poincaré section with \(E = 40\) is illustrated in Fig. 1, where the nonlinear interaction starts to generate a typical structure which is not dominated by the concentric circles alone. There appear five kinds of regular motion: three regular motions expressed by the innermost, middle, and outermost concentric circles, and two additional regular motions by inner four-crescent and outer four-crescent structure. Although the separatrix lines are not explicitly shown in Fig. 1, each four-crescent structure is surrounded by a respective separatrix. The elliptic point is situated just at the center of the crescent, whereas the hyperbolic point is at the edge of crescent island.

Applying the Lie transformation with the Deprit perturbation method in Sec. III to the Hamiltonian in Eq. (4.11), one obtains an analytic expression of the maximum integrable-form Hamiltonian, which contains information on the nonlinear resonant condition (4.3). By further applying the canonical transformation in Eq. (4.6), and by using the condition (4.9), one gets an analytic expression for the fixed points caused by the nonlinear resonance. The fixed points thus obtained in the first-order Deprit perturbation are plotted on the Poincaré section map in Fig. 1. As is recognized from Fig. 1, the first-order perturbation treatment of the present method already gives us an isolated resonant structure of the TDHF phase space, which is not simply understood in terms of the structure of the potential energy surface. In this way, one may get analytic information on the local constant of motion specific for each nonlinear island.

**V. SINGLE-PARTICLE DYNAMICS ASSOCIATED WITH THE NONLINEAR RESONANCE**

The structure of the TDHF manifold has been so far discussed through the numerical simulation of the TDHF trajectories [30]. In order to relate the nonlinear dynamics between the collective and single-particle modes of motion (in the level crossing region) with the nonlinear resonance in the TDHF manifold, however, it is...
decisive to make clear analytically what happens in the TDHF wave function in association with the nonlinear resonance.

To this aim, we introduce a set of the following one-body operators (with respect to \((\hat{J}_k, \phi_k)\)) which relates the canonical dynamics in the TDHF manifold with the single-particle dynamics in the maximal integrable-form representation;

\[
\hat{\phi}_k \equiv \frac{i}{\partial \hat{J}_k} e^{-i\hat{F}}, \quad \hat{\phi}_k \equiv i \frac{\partial \phi_k}{\partial \hat{J}_k} e^{-i\hat{F}}, \tag{5.1}
\]

where \(\hat{F}\) is defined in Eq. (2.5) and \((f, f^\mu_\nu)\) in \(\hat{F}\) are regarded as functions of the action-angle variables \((\hat{J}_k, \phi_k)\) in the maximal integrable-form representation, through the transformations Eqs. (2.8), (2.9), and (3.2). The single-Slater-determinant state \(|\hat{F}\rangle = \exp\{\hat{F}\}\langle \phi_0|\) in Eq. (2.5) thus becomes a function of \((\hat{J}_k, \phi_k)\) and is expressed as

\[
|\hat{F}\rangle = |\hat{J}, \phi\rangle. \tag{5.2}
\]

As is easily proved \([31]\), the “action” and “angle” operators \((\hat{J}_k, \phi_k)\) satisfy the weak canonical commutation relations,

\[
\{\hat{J}, \phi\} |\hat{J}_l, \phi_l\rangle |\hat{J}, \phi\rangle = i\delta_{kl},
\]

\[
\langle \hat{J}, \phi|\hat{J}_l, \phi_l\rangle |\hat{J}, \phi\rangle = \langle \hat{J}, \phi|\hat{J}_l, \phi_l\rangle |\hat{J}, \phi\rangle = 0. \tag{5.3}
\]

With the aid of the set of action and angle operators \((\hat{J}_k, \phi_k)\), the TDHF equation (2.6) is expressed as

\[
\delta(\hat{J}, \phi)\hat{H} - \sum_k (\hat{\phi}_k \hat{J}_k - \hat{\phi}_k \hat{J}_k) |\hat{J}, \phi\rangle = 0. \tag{5.4}
\]

By taking variations in \(|\hat{J}, \phi\rangle\) with respect to \((\hat{J}_k, \phi_k)\) and by using the relations (5.3), Eq. (5.4) turns into the canonical equation of motion in the maximal integrable-form representation,

\[
\hat{\phi}_k = \frac{\partial H}{\partial \hat{J}_k}, \quad \hat{J}_k = \frac{\partial H}{\partial \phi_k}, \tag{5.5}
\]

where the Hamiltonian \(H\) is defined by

\[
H(\hat{J}, \phi) \equiv \langle \hat{J}, \phi|\hat{H}|\hat{J}, \phi\rangle \tag{5.6}
\]

and is equivalent to one given in Eq. (3.18).

To make the following discussion simple, let us adopt the system with two degrees of freedom which has been considered in the previous section. The Hamiltonian is then given by

\[
H(\hat{J}_1, \hat{J}_2; \phi_1, \phi_2) \equiv \langle \hat{J}, \phi|\hat{H}|\hat{J}, \phi\rangle = H_{\text{integ}}(\hat{J}_1, \hat{J}_2) + H_{\text{coup1}}(\hat{J}_1, \hat{J}_2; \phi_1, \phi_2). \tag{5.7}
\]

What we bear in mind is a local region of the TDHF manifold near the isolated nonlinear resonance point \((\hat{J}_1^{(0)}, \hat{J}_2^{(0)})\) satisfying the nonlinear resonant condition \((4.3)\). Corresponding to the canonical transformation \((4.7)\), in this case, one may introduce the one-body operators with respect to \((\hat{I}_1, \theta_1; I_2, \theta_2)\).

\[
\hat{\theta}_1 \equiv \frac{1}{i} \frac{\partial \hat{F}}{\partial \hat{I}_1} e^{-i\hat{F}} = \frac{\partial \hat{J}_1}{\partial \hat{I}_1} \frac{1}{i} \frac{\partial e^{i\hat{F}}}{\partial \hat{J}_1} e^{-i\hat{F}} = \phi_1,
\]

\[
\hat{J}_1 \equiv \frac{i}{\partial \theta_1} e^{i\hat{F}} = \frac{\partial \phi_1}{\partial \theta_1} \frac{i}{\partial \phi_1} e^{-i\hat{F}} + \frac{\partial \phi_2}{\partial \phi_1} \frac{\partial e^{i\hat{F}}}{\partial \phi_2} e^{-i\hat{F}} = \hat{J}_1 + \frac{\hat{J}_2}{s},
\]

\[
\hat{\theta}_2 \equiv \frac{1}{i} \frac{\partial \hat{F}}{\partial I_2} e^{-i\hat{F}} = s\phi_2 - r\phi_1, \quad \hat{I}_2 \equiv \frac{i}{\partial \theta_2} e^{-i\hat{F}} = \hat{J}_2. \tag{5.8}
\]

They satisfy the weak canonical commutation relations

\[
\langle I, \theta|\{\hat{\theta}_i, \hat{J}_j\}|I, \theta\rangle = i\delta_{ij},
\]

\[
\langle I, \theta|\{\hat{\theta}_i, \hat{\theta}_j\}|I, \theta\rangle = \langle I, \theta|\hat{I}_i, \hat{I}_j\rangle|I, \theta\rangle = 0, \quad (i \text{ and } j = 1, 2) \tag{5.9}
\]

where the single-Slater-determinant state defined in Eq. (5.2) is expressed as a function of \((I_1, \theta_1; I_2, \theta_2)\),

\[
|I, \theta\rangle = \langle \hat{J}(I, \theta), \phi(\hat{I}, I, \theta)\rangle. \tag{5.10}
\]

In the nonlinear resonance region under consideration, as is seen from Eq. (4.8), the transformed Hamiltonian \(H(I, \theta, \phi(I, \theta)) \equiv \langle I, \theta|\hat{H}|I, \theta\rangle\) is \(\theta_1\) independent, and there holds a relation

\[
0 = \frac{\partial H}{\partial \theta_1} = \frac{\partial}{\partial \theta_1} \langle I, \theta|\hat{H}|I, \theta\rangle = \langle I, \theta|\hat{H}, \hat{I}_1\rangle|I, \theta\rangle. \tag{5.11}
\]

Equation (5.11) demonstrates that, in the local region near the nonlinear resonant point, \(I_1\) becomes a constant of motion and the corresponding generator \(\hat{I}_1\) can be regarded as a weak conserved quantity specifying a dynamical symmetry of the Hamiltonian operator. Thus, as already mentioned in Sec. IV, the new variables \((I_1, \theta_1)\) describe the new collective modes of motion transfigured from the old one with \((\hat{J}_1, \phi_1)\).

The stationary condition (4.9) is now rewritten as

\[
\frac{\partial H}{\partial I_2}(I_2^{(0)}, \phi_2^{(0)}) = \langle I, \theta|\hat{H}, \hat{I}_2\rangle|I, \theta\rangle = 0, \tag{5.12}
\]

Equations (5.11) and (5.12) clearly display that there exists a new type of stable single-Slater-determinant states in the nonlinear resonant region:

\[
|I, \theta|_{(I_2^{(0)}, \phi_2^{(0)})} \equiv |I_1, \theta_1; I_2^{(0)}, \phi_2^{(0)}\rangle, \tag{5.13}
\]

which is specified by a given value of \(I_1\) and elliptic (sta-
ble) fixed point \((l_2^{(0)}, \theta_2^{(0)})\) in the \(l_2-\theta_2\) phase plane, with an arbitrary value of \(\theta_1\).

It is worthwhile to mention that the new type of dynamical stable single-Slater-determinant state specified by Eqs. (5.11) and (5.12) is just associated with the elliptic fixed point \((l_2^{(0)}, \theta_2^{(0)})\) in the nonlinear resonant region, and is not reached by the usual static HF, CHF, or ATDHF theories [32]. Stabilization of the dynamical stable states is caused by the nonlinear resonant structure. This mechanism of stabilization may give us a new scope for understanding a variety of collective side-band structure, shape coexistence phenomena, etc. Since one may expect many fixed points in the TDHF manifold, one may also have a variety of stable and unstable resonant mean fields which have not been discovered yet.

VI. SUMMARY AND DISCUSSION

In order to try to open a new way of exploring the mutual dynamical dependence between the single-particle and collective modes of motion near to the level crossing region, in this paper, a general method is proposed to analytically investigate the nonlinear resonant structure of the TDHF manifold, without depending on the adiabatic assumption. In this method, the maximal integrable-form representation of the TDHF manifold plays an essential role. The representation is obtained within the general framework of the Lie transformation method with the Deprit perturbation treatment, by exploiting the recent progress in the theory of nonlinear dynamical system. As is always the case for any representation of the general manifold, the maximal integrable-form representation is also a local one which is specific for the starting HF state \(|\phi_0\rangle\). Provided that the local representation is obtained by extending the RPA solutions around \(|\phi_0\rangle\), the Lie transformation method with the Deprit perturbation method (in the theory of nonlinear dynamical system) is applicable. It is discussed that the representation provides us with analytic understanding of the nonlinear resonant structure of the TDHF manifold. The structure of the TDHF wave function in the nonlinear resonant region is investigated, with the purpose of trying to relate the nonlinear resonance in the TDHF manifold with the dynamics between the collective and single-particle modes of motion near the level-crossing region. The isolated nonlinear resonance in the TDHF manifold generates a new type of dynamical stable single-Slater-determinant states, which are topologically different from the TDHF states near the HF ground state \(|\phi_0\rangle\), and are not accessible by the usual static HF, CHF, or ATDHF theories. The new type of states in the nonlinear resonant region are characterized by a local constant of motion (dynamical symmetry), which can be regarded as a transfigured collective motion. The appearance mechanism of the new type of stable states gives us a new clue for understanding the occurrence mechanism of a variety of collective sideband structure, shape coexistence phenomena, etc. Structure of the single-particle states in the new type of stable states will be discussed in a separate paper in association with the topological phase.

In this paper, we have discussed how to study the rich structure of the TDHF manifold by confining ourselves to a case where only one HF state dominates. In order to study what is happening in the level crossing region, one has to further explore a case where at least two HF states play a role in characterizing the structure of the TDHF manifold. This subject will be discussed in a subsequent paper.

(1954).


