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*Invited talk presented by F. S. at the Symposium on "Harmony in Physics" (Philadelphia, May 1994) dedicated to Spatak Belyaev in honor of his seventies birthday.

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Abstract

To understand exceedingly rich structure of quantum excited states in the nuclei, an importance of exploring the complex structure of the time-dependent Hartree-Fock (TDHF) manifold is discussed. It is shown that various ideas developed in the general theory of nonlinear dynamics (e.g., the nonlinear resonance, elliptic and hyperbolic fixed points, order-to-chaos transition, etc.) play a decisive role in obtaining an analytic information on the quantum excited states, provided that the corresponding TDHF-manifold has a simple potential energy surface (PES) with only one minimum. When the TDHF-manifold has a PES with more than two local minima, one is involved into an important problem related with the adiabatic versus diabatic collective potentials. The adiabatic collective potential is usually obtained when one numerically solves the constrained Hartree-Fock (CHF) equation within a constraining coordinate space, which has a limited number of degrees of freedom. To explore dynamical relation between the adiabatic and diabatic single-particle states, one has to analyze the CHF-method within the full TDHF-manifold, which includes the constraint coordinate space. It turns out that the solutions of the CHF equation give many differentiable surfaces in the TDHF-manifold. By using differentiable property of the CHF solutions in the TDHF-manifold, a new method for reaching various HF points is discussed.

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1 Introduction

Phase transition in the nucleus has quite different aspects in comparison with that in the infinite system. The important subjects in developing the quantum theory in such a finite many-body system as nuclei are to analytically understand the following points; a) how a set of good quantum numbers specifying a certain group of collective excited states undergoes a change as they develop into the large-amplitude region far from the ground state, b) how there appears a new type of collective excited states characterized by another local set of good quantum numbers, and c) why there dominate the excited states which have no good quantum numbers as the system gets more energy. Within the framework of the time-dependent Hartree-Fock (TDHF) theory, the above problems require a new general theory capable of describing what kinds of dynamical change will take place in the adiabatic invariants (AI) (instead of the good quantum numbers) characterizing the corresponding collective TDHF trajectories when they develop into the large-amplitude region far from a certain stable mean-field. Since the basic equation of the TDHF-theory is known to be formally equivalent to the Hamilton equations of motion for a classical system with many degrees of freedom[1], and since it has been one of the main objectives of the general theory of nonlinear dynamics (GTND) to analytically understand how the AI characterizing each trajectory undergo a change depending on its amplitude[2], it may be important to exploit various ideas of the GTND in developing the theory of large-amplitude nuclear collective motion. In §2, a relation between the nuclear collective dynamics within the TDHF theory and the nonlinear dynamics will be discussed.

According to a recent development in the nuclear structure physics especially in the high-spin physics, it has been clarified that there often coexist many stable mean-fields with different geometrical shapes (β_2 , γ , β_4 , Δ , ω , ...) in one nucleus[3]. For example, there coexist the normal prolate, super prolate and normal oblate deformations in ^{152}Dy , where the superdeformed band had been first observed. It has been recognized that various nuclear collective modes and associated deformation could be attributed to specific symmetries of the *intrinsic* Hamiltonian[4]. However, the stable mean-fields characterizing different intrinsic states and different phases in the nucleus are not necessarily orthogonal with one another, unlike a case with the infinite system. It is thus imperative to explore mutual relation among various stable mean-fields, dynamical role of adiabatic and diabatic single-particle states, microscopic derivation of the potential energy surface (PES) with and without configuration constrained, microscopic origin of the topological phase, etc. Since these points are related to the mean-field aspect of the nuclear many-body problem, they are supposed to be explored within the TDHF theory.

To study the microscopic relation between different stable mean-fields, one has to start with developing a new numerical method which is capable of finding out many local minima and maxima for a given nuclear Hamiltonian. Applying the numerical method of calculating the constrained (C-)HF equation by either using the nonlinear eigenvalue equation

or the gradient method[5] (with the adiabatic requirement), however, one only gets an adiabatic collective potential as well as the adiabatic single-particle states satisfying the non-crossing rule. Since this method is only picking up the most energetically favorable state under a given constraining condition, many HF points are eventually discarded. In §3, the conventional numerical CHF method is investigated within the TDHF-manifold, and a new numerical method for obtaining various HF-point characterized by different intrinsic configuration will be proposed.

2 Basic Idea of the General Theory of Nonlinear Dynamics

2.1 Structure of the TDHF-Manifold

Since we are interested in the mean-field aspect of the nuclear many-body problem, we start with the TDHF equation

$$\delta\langle\phi|\hat{H} - id/dt|\phi\rangle = 0, \quad |\phi\rangle = \exp \hat{F}|\phi_0\rangle, \quad (1)$$

where $|\phi_0\rangle$ means a certain HF state satisfying $\delta\langle\phi_0|\hat{H}|\phi_0\rangle = 0$, and the convention $\hbar = 1$ is applied here and hereafter. By means of the particle and hole operators $\hat{a}_\mu^\dagger$ and $\hat{b}_i^\dagger$ with respect to $|\phi_0\rangle$ where μ and i denote the particle and hole single-particle states, the general time-dependent one-body anti-Hermitian operator $\hat{F}$ in Eq.(1) is expressed as

$$\hat{F} = \sum_{\mu i} \{f_{\mu i} \hat{a}_\mu^\dagger \hat{b}_i^\dagger - h.c.\}. \quad (2)$$

It is well known that the TDHF equation (1) is reduced to Hamilton's canonical equations of motion

$$i\dot{C}_{\mu i} = \frac{\partial H}{\partial C_{\mu i}^*}, \quad i\dot{C}_{\mu i}^* = -\frac{\partial H}{\partial C_{\mu i}}; \quad H \equiv \langle\phi|\hat{H}|\phi\rangle, \quad C_{\mu i} \equiv (f \frac{\sin \sqrt{f^\dagger f}}{\sqrt{f^\dagger f}})_{\mu i} \quad (3)$$

which shows the symplectic structure of the TDHF-manifold $C_{\mu i}$, $C_{\mu i}^*$.

Here we summarize the basic ideas of the GTND in a form appropriate for the nuclear collective motion. Its essential points have been mainly discussed by using the classical system with two degrees of freedom $H(x_1, p_1; x_2, p_2)$ or with 1.5 degrees of freedom like the kicked rotor system. A schematic Poincaré section map at (x_1, p_1) -plane is illustrated in Fig.1 for the case with small nonlinear effects. When the nonlinear effects are sufficiently small, as is shown in Fig.1a, the Poincaré section map is dominated by only the concentric circles whose centers are located at the origin of the $(x_1, p_1; x_2, p_2)$ -coordinate system. This

Figure 1: Schematic illustration of Poincaré section map for the case with small nonlinear effects.

means that there exists only one type of motion characterized by a single set of *global* AI. When the nonlinear effects start to act, there appears a nonlinear resonant island depicted in Fig.1b. The objective of the GTND has been to disclose the order-to-chaos transition mechanism by analytically understanding approximate AI, i.e., approximate *local* constants of motion of each trajectory. In the course of this study, it turned out to be decisive to introduce the *most natural coordinate system*[2] for each trajectory. If one wants to know an analytic form of the AI of the trajectory belonging to the resonant island, it is natural to employ the coordinate system $(\tilde{x}_1, \tilde{p}_1; \tilde{x}_2, \tilde{p}_2)$ whose origin is situated at the resonant elliptic fixed point, rather than to employ the coordinate system $(x_1, p_1; x_2, p_2)$.

Let us briefly discuss how to get an analytic information of the AI for each trajectory. To this end, it is convenient to employ the action-angle representation $(I_1, \theta_1; I_2, \theta_2)$ instead of the coordinate-momentum representation; $x_i = \sqrt{I_i} \cos \theta_i$, $p_i = \sqrt{I_i} \sin \theta_i$; $i = 1$ and 2 . The Hamiltonian is then represented as,

$$H(I_1, \theta_1; I_2, \theta_2) = H_0(I_1; I_2) + H_{int}(I_1, \theta_1; I_2, \theta_2). \quad (4)$$

Here, the action variables I_1 and I_2 , as well as the integrable part of the Hamiltonian $H_0(I_1; I_2)$ are determined by using the conventional RPA, whereas $H_{int}(I_1, \theta_1; I_2, \theta_2)$ represents the anharmonic (non-linear) terms. The I_1 and I_2 are then regarded as the AI specifying the trajectory which is running near the origin of the coordinate system $(x_1, p_1; x_2, p_2)$, representing the small-amplitude vibrational motion. To get slightly different AI denoted by I'_1 and I'_2 that characterize the trajectory running in a region relatively far away from the origin, one has to obtain a new integrable Hamiltonian $H'_0(I'_1, I'_2)$, by properly taking account of the anharmonic effects H_{int} *perturbatively*. Applying the classical perturbation

theory, one gets a new representation of the Hamiltonian,

$$H = H'_0(I'_1, I'_2) + H'_{int}(I'_1, \theta'_1; I'_2, \theta'_2). \quad (5)$$

In this way, one may know how the AI undergoes a change as the amplitude of the trajectory from the origin increases. The analytic structure of the resultant I'_1 and I'_2 contain an information how the microscopic structure of the boson operator describing the collective excited states transfigures depending on the amplitude.

A general perturbation method for obtaining the most natural coordinate system (called the maximally-decoupled collective coordinate system) in the TDHF-manifold was first proposed by Marumori et al. under the name of the *self-consistent collective coordinate* (SCC) *method*[6]. By using the Birkoff-Gustavson normal form expansion[7], the SCC method was further developed in a form that is suitable for defining the adiabatic invariants I'_1 and I'_2 perturbatively by starting from I_1 and I_2 [8]. Here it should be noticed that the physical boson expansion method developed by A. Klein[9] just rests on this line.

The above classical perturbative treatment can not be applied any more when there holds the following *resonant* condition;

$$r \frac{\partial H'_0(I'_1, I'_2)}{\partial I'_1} - s \frac{\partial H'_0(I'_1, I'_2)}{\partial I'_2} = 0, \quad r \text{ and } s \text{ are prime numbers.} \quad (6)$$

However, the condition (6) tells us an analytic information on a pair of hyperbolic and elliptic resonant fixed points. Namely, one gets an analytic form of the canonical transformation $(I'_1, \theta'_1; I'_2, \theta'_2) \Leftrightarrow (\tilde{I}_1, \tilde{\theta}_1; \tilde{I}_2, \tilde{\theta}_2)$: $\tilde{I}_1 = I'_1 - rI'_2$, $\tilde{I}_2 = sI'_2$, $\tilde{\theta}_1 = \theta'_1$, $\tilde{\theta}_2 = (\theta'_2 + r\theta'_1)/s$, which provides us with a new representation of the Hamiltonian in the resonant region,

$$H = \tilde{H}_0(\tilde{I}_1; \tilde{I}_2) + \tilde{H}_{int}(\tilde{I}_1, \tilde{\theta}_1; \tilde{I}_2, \tilde{\theta}_2). \quad (7)$$

Knowing the Hamiltonian in Eq.(7) expressed by the *primary resonant coordinate system* $(\tilde{I}_1, \tilde{\theta}_1; \tilde{I}_2, \tilde{\theta}_2)$, one may repeat the same perturbative procedure as before to analytically obtain slightly different AI, $\tilde{I}'_1$ and $\tilde{I}'_2$ of the trajectory which is running in a region relatively far from the primary resonant elliptic fixed point, until one comes across a new resonant condition indicating a set of new fixed points of the secondary resonant island, which surrounds the primary resonant island.

In this way, one may disclose why a set of AI characterizing the trajectory running near a certain potential minimum undergoes a change as the amplitude of the trajectory increases, and how a new set of local constants of motion is generated under the influence of nonlinear resonance as the system gets more energy.

The general perturbation method to disclose complex resonant structure of the TDHF-manifold has been developed[10] by using the Lie transformation with the Deprit perturbation method[2]. In order to visualize feasibility of the theory, we adopt a modified SU(3)

model Hamiltonian

$$\hat{H} = \sum_{i=0}^2 \varepsilon_i \hat{K}_{ii} + \sum_{i=1}^2 \frac{V_i}{2} (\hat{K}_{i0} \hat{K}_{i0} + h.c.), \quad \hat{K}_{ij} \equiv \sum_{m=1}^N \hat{c}_{im}^\dagger \hat{c}_{jm}. \quad (8)$$

There are three N-fold degenerate levels with $\varepsilon_0 < \varepsilon_1 < \varepsilon_2$. In a case with an even N-particle system, a time-dependent single Slater-determinant $|\phi\rangle$ in Eq.(1) is given by

$$\begin{aligned} |\phi\rangle &\equiv e^{\hat{F}} |\phi_0\rangle (= |x_1, p_1, x_2, p_2\rangle); \\ |\phi_0\rangle &\equiv \prod_{m=1}^N \hat{c}_{0m}^\dagger |0\rangle, \quad \hat{F} = \sum_{i=1}^2 \{f_i \hat{K}_{i0} - h.c.\}, \\ p_i &\equiv \frac{i}{\sqrt{2}} (c_i^* - c_i), \quad x_i \equiv \frac{1}{\sqrt{2}} (c_i^* + c_i), \\ c_i &\equiv \sqrt{N} f_i \sin |f|/|f|, \quad |f| \equiv \sqrt{\sum_{k=1}^2 f_k^* f_k}, \end{aligned} \quad (9)$$

where $|\phi_0\rangle$ satisfies the HF condition $\delta\langle\phi_0|\hat{H}|\phi_0\rangle = 0$. One then obtains the classical Hamiltonian $H(x_1, x_2, p_1, p_2) \equiv \langle\phi|\hat{H}|\phi\rangle$ with two degrees of freedom.

In Fig.2, the nonlinear resonant elliptic and hyperbolic fixed points (center of crescent islands and intersection point of surrounding separatrix, respectively) obtained by our first order perturbation treatment are illustrated. Parameters used in the calculation are $N=30$, $\varepsilon_0 = 0$, $\varepsilon_1 = 1$, $\varepsilon_2 = 2$ and $V = -0.01$, and the Poincaré map is drawn for a case with total energy $E=40$. From Fig.2, it is recognized that an analytic information on the resonant structure obtained in our first order perturbation treatment already gives the basic structure of the TDHF-manifold. In this way, one may get an analytic information how the AI (local constants of motion) of the TDHF-trajectory changes depending on the energy, amplitude from the origin, etc.

It has been pointed out[10] that the resonant elliptic fixed point in the TDHF-manifold just corresponds to a new type of stable mean-field, which can not be reached by the usual HF, CHF nor adiabatic TDHF theories[10]. Since the AI, $\tilde{I}_1$ and $\tilde{I}_2$ have a sense in the resonant region in the TDHF-manifold, they are regarded as local constants of motion associated with the *dynamical symmetry* realized near the resonant island.

2.2 Structure of the Quantum States of Many-Fermion System

The above idea is naturally generalized to the full-quantum treatment of the nuclear system; What is discussed in the microscopic theory of nuclear collective motion is how the microscopic structure of a collective phonon operator characterizing the collective vibrational states transfigures under the effects of anharmonic interaction when it develops into

Figure 2: Elliptic and hyperbolic points obtained by the SCC method are denoted by solid circle and solid triangle. Taken from Ref.[10].

the large-amplitude region, why there appears another side-band structure of the collective motion specified by new local good quantum numbers as the system gets more energy, and why there appears a set of eigenstates whose nearest-neighbor level-spacing statistics is well reproduced by the random matrix theory.

The quantum SCC method[11] has been developed under dictation what was developed in the TDHF-manifold summarized in the previous subsection. In this theory, the fermion system is first transformed into the boson system by using the boson expansion method. In the present case, it is achieved by introducing the boson operators $[B_i, B_j^\dagger] = \delta_{ij}$, $[B_i, B_j] = 0$; $(i, j = 1, 2)$. Then, the eigenstates $\{|\lambda\rangle\}$ of the Hamiltonian are obtained by diagonalizing it within the boson representation of the fermion system. The structure of eigenstate $|\lambda\rangle$ is visualized by introducing a profile function[12] defined through

$$G^\lambda(x_1, p_1) \equiv \int dp_2 F^\lambda(x_1, p_1; x_2 = 0, p_2),$$

$$F^\lambda(x_1, p_1; x_2, p_2) \equiv |(c_1, c_2|\lambda)|^2, \quad (10)$$

where $|c_1, c_2\rangle = |x_1, p_1; x_2, p_2\rangle$ denotes the boson coherent state given by

$$|c_1, c_2\rangle \equiv \exp \sum_{i=1}^2 \{c_i B_i^\dagger - h.c.\} |0\rangle;$$

$$p_i \equiv \frac{i}{\sqrt{2}}(c_i^* - c_i), \quad x_i \equiv \frac{1}{\sqrt{2}}(c_i^* + c_i). \quad (11)$$

By using a trivial correspondence between the TDHF state and the coherent state given by $|x_1, p_1; x_2, p_2\rangle \Leftrightarrow |x_1, p_1; x_2, p_2\rangle$, the profile function (10) is expressed in the TDHF-manifold. They are thus regarded as a quantum correspondent of the Poincaré section map of the TDHF trajectories, and are illustrated in Fig.3. Similarity between the profile

functions and the Poincaré section map is remarkable; Figs.3a and 3f show the same structure as the outer most and inner most concentric circles in Fig.2. Figs.3b and 3c correspond to the elliptic and hyperbolic points of the inner four-crescent nonlinear resonant islands in Fig.2, and Figs.3d and 3e are quantum correspondents of the fixed points associated with the outer four-crescent islands. The eigenstate whose profile function has the same structure as that of resonant points in Fig.2 turned out to be regarded as a *quantum nonlinear resonant state*[12] characterized by a set of local good quantum numbers, like the classical nonlinear resonance by the local adiabatic invariant. As is seen from the above example, an analytic understanding of the TDHF-manifold is very important in studying the complex structure of the quantum many-fermion space in the large-amplitude region, and in obtaining a set of approximate good quantum numbers which specifies each eigen state. In this way, one may study exceedingly rich structure of the quantum excited states of the many fermion system.

3 Structure of the TDHF-Coordinate Space with Many Local Minima

3.1 Adiabatic and Diabatic Single-Particle States

We have so far discussed the structure of the TDHF-manifold governed by the simple potential which has only one minimum. As mentioned in the introduction, however, one has to extend the method discussed in the previous section to the more general TDHF-manifold whose potential has many local minima. In this case, one is inevitably involved into various theoretical issues related to the adiabatic vs. diabatic single-particle basis states.

According to Hill-Wheeler's picture[13], the collective motion feels the diabatic potential when its speed is sufficiently rapid, whereas it feels the adiabatic potential (envelop of the diabatic potentials) when it is slow enough. This picture is essentially derived from the Born-Oppenheimer approximation (BOA) in the molecular physics. In the nuclear physics, however, the BOA is by no means trivial. To discuss the above mentioned issues, it is instructive to start with reviewing how the adiabatic and diabatic collective potential are microscopically introduced in the nuclear physics. According to the conventional numerical method of the CHF equation or its approximation through the Nilsson-Strutinsky method, one is only interested in the most energetically favorable single Slater-determinant state (adiabatic requirement) for a given constraining condition $\langle \hat{Q} \rangle = q$, because it has been not easy problem to numerically find out many local minima satisfying the HF condition within the large dimensional parameter space. Since it is much easier to find the most energetically favorable state by employing a numerical program based on the gradient method, one may obtain the adiabatic collective potential, as well as the adiabatic single-particle states

Figure 3: Profile function of various eigenstates. The eigenenergies are $E_\lambda \approx 40$ and are nearly the same as that of the semi quantum system in Fig.2. Taken from Ref.[12].

Figure 4: Adiabatic and diabatic potential. Taken from Ref.[13].

satisfying the non-crossing rule.

On the other hand, there have been proposed many practical methods called "diabatic recipe," which intend to phenomenologically introduce the diabatic single-particle states so as to explain the experimental data. After Hamamoto's suggestion on an inadequacy of the cranking model near the level crossing region in the high spin physics[14], the diabatic base is usually introduced by keeping the single-particle configuration of the intruder orbit unchanged. In practice, this base is constructed by using a fairly general method of eliminating a so-called "virtual interaction", which appears in a small region near the single-particle level crossing point[15]. In the heavy-ion deep-inelastic collision, Nörenberg[16] has developed the dissipative diabatic dynamics by introducing the diabatic base, which is defined in such a way that the nodal structure of the single-particle wave functions are kept unchanged during the reaction process.

The basic idea of employing the diabatic base is related with an existence of various intrinsic states, which may be associated with different types of collective motion. Since the different intrinsic states are characterized by different single-particle configurations within the independent-particle approximation, and since the intrinsic state is supposed to be unchanged within the same band structure of collective excited states, one may introduce the diabatic base by regarding the single-particle configuration as an approximate good quantum numbers.

Recently, Bengtsson-Nazarewicz[17] have pointed out superiority of the diabatic potential over the adiabatic one. When they apply the usual adiabatic Nilsson-Strutinsky method to the collective potential near the ground state in the neutron deficient Pb-isotopes, they get the adiabatic PES which has small shoulder in the oblate region. When they apply the

Figure 5: Adiabatic and diabatic potential for neutron deficient Pb-isotopes. Taken from Ref.[17].

diabatic recipe developed in the high spin physics to this particular deformation problem, they obtain three diabatic potentials; the lowest spherical potential, the next lowest oblate potential and occasionally the third lowest prolate potential. As is shown in Fig. 5, they found that the local minimum of the oblate diabatic potential well reproduce the systematic behavior of the excited 0^+ state in the neutron deficient Pb-isotopes. They clarified that the ACHF solution does not always give a sufficient information on the nuclear excited states, and a particle number of the intruder orbits may play a role of an approximate good quantum number in characterizing the excited states.

Since the various intrinsic states are characterized by the stable HF-points, it is of special importance to develop a new numerical method to find many local minima and many saddle points satisfying the HF condition without depending on the diabatic recipe. For this aim, it is decisive to study the CHF method within the TDHF-coordinate space $\{x_{\mu i}\}$. Here, $x_{\mu i}$ is defined from Eq.(3) by

$$x_{\mu i} \equiv \frac{1}{\sqrt{2}}(C_{\mu i}^* + C_{\mu i}), \quad p_{\mu i} \equiv \frac{i}{\sqrt{2}}(C_{\mu i}^* - C_{\mu i}). \quad (12)$$

On the other hand, the constraining coordinate space $\{q\}$, is introduced by the expectation value of a limited number of constraining operators $q = \langle \phi | \hat{Q} | \phi \rangle$ where the CHF method is usually formulated. Since $\{x_{\mu i}\}$ gives a complete description of the TDHF-coordinate space whereas $\{q\}$ does not, the CHF method without adiabatic requirement is expected to be elucidated within $\{x_{\mu i}\}$.

Let us take a simple model Hamiltonian[18] given by

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{H}_V + \hat{H}_Y, \quad \hat{H}_0 = \varepsilon_0 \hat{K}_{00} + \varepsilon_1 \hat{K}_{11} + \varepsilon_2 \hat{K}_{22}, \\ \hat{H}_V &= \frac{V_1}{2}(\hat{K}_{10} \hat{K}_{10} + h.c.) + \frac{V_2}{2}(\hat{K}_{20} \hat{K}_{20} + h.c.), \end{aligned}$$

$$\begin{aligned} \hat{H}_Y &= V_3\{\hat{K}_{10}(\hat{K}_{11} + \hat{K}_{22}) + h.c.\} + V_4\{\hat{K}_{10}(\hat{K}_{12} + \hat{K}_{21}) + h.c.\} \\ &+ V_5\{\hat{K}_{20}(\hat{K}_{11} + \hat{K}_{22}) + h.c.\} + V_6\{\hat{K}_{20}(\hat{K}_{12} + \hat{K}_{21}) + h.c.\}, \end{aligned} \quad (13)$$

which is the same as the Hamiltonian in Eq.(8) except for $\hat{H}_Y$ interaction. In this model, we also consider an even N-particle system. As a constraining operator, we take the most general one-body Hermitian operator as

$$\begin{aligned} \hat{Q} &= Q_{1x}(\hat{K}_{10} + h.c.) + Q_{1y}(\hat{K}_{20} + h.c.) + \\ &Q_{2x}\hat{K}_{11} + Q_{2y}\hat{K}_{22} + Q_3\hat{K}_{00} + Q_4(\hat{K}_{21} + h.c.). \end{aligned} \quad (14)$$

In the present case, the general single-Slater determinant $|\phi\rangle$ in Eq.(1) is expressed by Eq.(9). To numerically obtain many local minimum and maximum points of the PES in the TDHF-coordinate space, one usually employs the CHF method. It often happens in the realistic CHF calculation that an appreciable change in the occupation probability takes place only in a few single-particle orbits when one pays attention to a tiny region of the constraining variables. In other words, a strong mixture among many single-particle orbits that stabilizes a new self-consistent mean-field may be mainly induced by many sequential local rearrangements that involves only a few single-particle orbits. Then the above simple model Hamiltonian is expected to simulate local situation appearing in the realistic CHF calculation.

The matrix representation of the density matrix $\rho_{ij} = \langle \phi | \hat{K}_{ji} | \phi \rangle$ and the CHF one-body Hamiltonian for the single-Slater determinant $|\phi\rangle$ are expressed as

$$\begin{aligned} \hat{\rho} = \sum_{ij} \rho_{ij} \hat{K}_{ij} &\Rightarrow \rho = \frac{1}{2} \begin{pmatrix} x_2^2 & x_1 x_2 & \gamma x_2 \\ x_1 x_2 & x_1^2 & \gamma x_1 \\ \gamma x_2 & \gamma x_1 & 4\gamma^2 \end{pmatrix}, \\ \gamma &= \sqrt{(N - (x_2^2 + x_1^2)/2)/2}. \end{aligned} \quad (15)$$

$$\begin{aligned} \{\hat{H} - \lambda \hat{Q}\}_{\text{one-body}} &\Rightarrow \mathcal{H} = e^{-F} h e^F, \quad h_{ij} = \frac{\partial(V - \lambda Q)}{\partial \rho_{ji}}, \quad (i,j=0,1 \text{ and } 2), \\ V(x_1, x_2) &= \langle \phi | \hat{H} | \phi \rangle, \quad Q(x_1, x_2) = \langle \phi | \hat{Q} | \phi \rangle. \end{aligned} \quad (16)$$

The basic equations of the CHF method is given by

$$\delta \langle \phi | \hat{H} - \lambda \hat{Q} | \phi \rangle = 0, \quad \langle \phi | \hat{Q} | \phi \rangle = q. \quad (17)$$

In the TDHF-coordinate space, the first equation in Eq.(17) is simply expressed as

$$\frac{\partial V}{\partial x_1} = \lambda \frac{\partial Q}{\partial x_1}, \quad \frac{\partial V}{\partial x_2} = \lambda \frac{\partial Q}{\partial x_2}, \quad (18)$$

which is equivalent to $\mathcal{H}_{20} = \mathcal{H}_{10} = 0$.

Figure 6: Contour map of the a) potential $V(x_1, x_2)$, and b) constrained coordinate $Q(x_1, x_2)$. Taken from Ref.[18].

To understand what happens in the usual numerical calculation of the CHF equation based on the adiabatic requirement, it is desirable to divide the CHF equation (17) into two parts in the TDHF-coordinate space. From the first equation in Eq.(17), i.e., from Eq.(18), one gets

$$0 = \frac{\partial V}{\partial x_2} \frac{\partial Q}{\partial x_1} - \frac{\partial V}{\partial x_1} \frac{\partial Q}{\partial x_2}, \quad (19)$$

by eliminating the Lagrange multiplier λ . Equation (19) defines *differentiable lines* in $\{x_1, x_2\}$, which is the most important property of the CHF solution when one analyzes it within the TDHF coordinate space. However, this differentiable nature is not considered in the usual numerical method of the CHF within the constraining coordinate space. Equation (18) is then used to get a concrete value of the Lagrange multiplier at each point on the resultant lines. By means of the second CHF equation, i.e., the constraining condition given by $Q(x_1, x_2) = q$, one obtains a *many-to-one* transformation $\{x_1, x_2\} \rightarrow \{q\}$, i.e., from $\{x_1, x_2\}$ to the constraining coordinate space $\{q\}$.

In Fig. 6, the contour maps of $V(x_1, x_2)$ and $Q(x_1, x_2)$ in $\{x_1, x_2\}$ are illustrated. A set of parameters used in the present numerical calculation is: $N = 4, \varepsilon_0 = 0, \varepsilon_1 = 16.4, \varepsilon_2 = 18, V_1 = V_2 = -16/3, V_3 = -4/15, V_4 = -2/15, V_5 = 0, V_6 = -8/3, Q_{1x} = 1, Q_{1y} = 1/5, Q_{2x} = Q_{2y} = 2$ and $Q_3 = Q_4 = 0$. The parameters in the Hamiltonian are chosen in such a way that the system has more than two local minima besides the trivial HF-point $|\phi_0\rangle$, and there exist neighboring two saddle points. Within the region shown in Fig. 6, there are three stable HF-points (denoted by $|\phi_0\rangle, |\phi_1\rangle$ and $|\phi_2\rangle$) and two unstable HF-points (saddle points denoted by $|\phi_3\rangle$ and $|\phi_4\rangle$). In a region near to $x_1^2 + x_2^2 = 2N$

Figure 7: Potential energy in $\{q\}$ -space. Taken from Ref.[18].

that is not included in Fig. 6, there are three other unstable HF-points (one saddle and two maxima) which are irrelevant to the following discussion. The parameters in the constraining operator are determined in such a way that the solution of Eq.(19) has more than two differentiable continuous lines. In Fig. 6, the solution of Eq.(19) are superimposed on the PES. These continuous lines (two of those are denoted by A and B) do not cross with each other and every HF-point rests on one of these lines.

By using the mapping $\{x_1, x_2\} \rightarrow \{q\}$, the potential energies on the line A and line B are transformed to $V_A(q)$ and $V_B(q)$ in the constraining coordinate space shown in Fig.7. As is seen from Figs.6 and 7, there are some region where the CHF equation has more than two solutions for one given value of q . To avoid this many-valuedness, one may pick up the most energetically favorable states for the given value of q by applying the adiabatic requirement so as to obtain an adiabatic PES $V_{adia}(q)$ in $\{q\}$. However, there are no dynamical reason to connect $V_A(q)$ and $V_B(q)$ at the crossing point where a condition $V_A(q) = V_B(q)$ is satisfied, because these two potentials belong to two different continuous lines in Fig.6. When one apply the adiabatic requirement in Fig.7, one can only find a small shoulder in $V_{adia}(q)$ without knowing a well developed second stable HF-point $|\phi_2\rangle$. This situation may describe what we met in Fig. 5, where the adiabatic potential shows only small shoulder in the oblate side.

3.2 Configuration Constrained Hartree-Fock Method

Let us consider how to reach the HF-state $|\phi_2\rangle$ situated on the line B starting from the line A. The contour map of the PES near the saddle points is shown in Fig. 8. As is seen from

Figure 8: PES in the TDHF-coordinate space near the saddle point. Taken from Ref.[18].

Fig. 8, these two lines may easily be varied by a subtle change of the PES near the saddle points. For example, it is shown in Fig. 9 how strongly the solution of Eq.(19) changes depending on the single-particle energy of the orbit $i = 1$.

As indicated by the diabatic recipe, one may get the diabatic CHF solution by keeping an occupation probability of some orbit constant. This procedure is practically achieved by eliminating the so-called virtual interaction near the single-particle level-crossing region[15]. In what follows, we examine this procedure by studying what happens in the TDHF-coordinate space. An introduction of a new method called the configuration (C-)CHF is achieved by first selecting an appropriate point $(x_1^{(0)}, x_2^{(0)})$ on the line A near the saddle point. In the present case, the particle number in the orbit 1 is kept constant on the vertical line (parallel to ordinates) with $x_1 = x_1^{(0)}$, while is the orbit 2 on the horizontal line (parallel to abscissas) with $x_2 = x_2^{(0)}$. (Note that the single-particle orbits specifying the configuration are not necessarily chosen for the state $|\phi_0\rangle$.) In the following, we discuss a case where the particle number in the orbit 1 is kept constant. Let us solve the first equation in Eq.(18) on the vertical line,

$$0 = \left(\frac{\partial V(x_1, x_2)}{\partial x_1} - \lambda_1 \frac{\partial Q(x_1, x_2)}{\partial x_1} \right) \Big|_{x_1=x_1^{(0)}}, \quad (20)$$

which defines $\lambda_1(x_1^{(0)}, x_2)$. Here it should be noticed that the condition (20) is equivalent to $\mathcal{H}_{10}(x_1^{(0)}, x_2) = 0$. When one inserts the resultant $\lambda_1(x_1^{(0)}, x_2)$ into $\mathcal{H}$, one gets $\mathcal{H}_{10}(x_1^{(0)}, x_2) = 0$ whereas $\mathcal{H}_{20}(x_1^{(0)}, x_2) \neq 0$ at almost every point on the vertical line. The

Figure 9: Drastic change of the CHF solution in the TDHF-coordinate space.

other equation in Eq.(18) on the vertical line is given by

$$0 = \left(\frac{\partial V(x_1, x_2)}{\partial x_2} - \lambda_2 \frac{\partial Q(x_1, x_2)}{\partial x_2} \right) \Big|_{x_1=x_1^{(0)}}, \quad (21)$$

which is equivalent to $\mathcal{H}_{20}(x_1^{(0)}, x_2) = 0$ and defines $\lambda_2(x_1^{(0)}, x_2)$. At the points (denoted by α and β in Fig. 8) where the vertical line intersects with the line B, there holds a relation

$$\lambda_1(x_1^{(0)}, x_2) = \lambda_2(x_1^{(0)}, x_2). \quad (22)$$

Equations (20-22) constitute the basic equations of the CCHF method, which provide us with a way how to reach the line B by starting from a certain point on line A near the saddle point. After reaching the point α (or β) where $\mathcal{H}_{10}(x_1^{(0)}, x_2) = \mathcal{H}_{20}(x_1^{(0)}, x_2) = 0$ is satisfied, one switches back to the usual CHF method to find another HF-point $|\phi_2\rangle$ on line B.

On the vertical line, $\{\hat{H} - \lambda\hat{Q}\}_{\text{one-body}}$ with $\lambda = \lambda_1(x_1^{(0)}, x_2)$ can not define the single-particle states because there holds $\mathcal{H}_{20}(x_1^{(0)}, x_2) \neq 0$ except for the intersection points. To define the single-particle states in between the points $(x_1^{(0)}, x_2^{(0)})$ and α (or β), one has to eliminate $\mathcal{H}_{20}(x_1^{(0)}, x_2)$ by regarding it as virtual interaction. In defining the single-particle states, there are two ways; to use $\lambda_1(x_1^{(0)}, x_2)$ with elimination of $\mathcal{H}_{20}(x_1^{(0)}, x_2)$, or to use $\lambda_2(x_1^{(0)}, x_2)$ with elimination of $\mathcal{H}_{10}(x_1^{(0)}, x_2)$. This ambiguity does not cause any trouble when one wants to reach the intersection point and to get the HF-point $|\phi_2\rangle$. An elimination of the virtual interaction thus effectively induces a subtle change in the PES so as to connect the line A with line B through the vertical line indicated in Fig.8. Since

Figure 10: CHF solution for ^{82}Sr with Skyrme interaction. Taken from Ref.[19].

the diabatic recipe in the Nilsson-Strutinsky method only discusses an effective one-body Hamiltonian simulating $\{\hat{H} - \lambda\hat{Q}\}_{\text{one-body}}$ in Eq.(16), various properties of the PES can be specified by only defining appropriate single-particle states, like the diabatic single-particle states under the diabatic recipe. From the above discussion, an elimination of some parts of particle-hole components in the effective one-body Hamiltonian is understood to be a practical method to jump over from one continuous line containing the HF ground state to another line that runs through another HF point, e.g., the excited 0^+ states in the neutron deficient Pb-isotopes.

In Fig.10, the CHF solution for ^{82}Sr with Skyrme interaction is shown[19]. Since we have exploit differentiable property of the CHF solution in the TDHF-coordinate space, we get many local minimum points.

In the present paper, we put special emphases on the relation between the adiabatic and diabatic single-particle states under the influence of the two-body particle-hole correlations. In order to discuss the realistic case, it is certainly necessary to include the effects coming from the particle-particle (pairing) correlations as well as the uniform rotation. However, it is important to explore these effects separately. Moreover, an inclusion of many local minima requires the full analysis of the gauge structure of the TDHF-manifold[20]. These subjects will be reported elsewhere.

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