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K. Iwasawa^a, F. Sakata^a, W. Nazarewicz^{b,c}, T. Marumori^d, and J. Terasaki^a

^a *Institute for Nuclear Study, University of Tokyo, Tanashi, Tokyo 188, Japan*

^b *Joint Institute for Heavy-Ion Research and Physics Division,
Oak Ridge National Laboratory, Oak Ridge, TN37831, USA*

^c *Institute of Theoretical Physics, Warsaw University,
ul. Hoza 69, PL-00-681 Warsaw, Poland*

^d *Department of Physics, Faculty of Science, Science University of Tokyo,
Tokyo 162, Japan*

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^a *Institute for Nuclear Study, University of Tokyo, Tanashi, Tokyo 188, Japan*

^b *Joint Institute for Heavy-Ion Research and Physics Division,
Oak Ridge National Laboratory, Oak Ridge, TN37831, USA*

^c *Institute of Theoretical Physics, Warsaw University,
ul. Hoża 69, PL-00-681 Warsaw, Poland*

^d *Department of Physics, Faculty of Science, Science University of Tokyo,
Tokyo 162, Japan*

Abstract

The structure of solutions of the constrained Hartree-Fock method is studied within the time-dependent Hartree-Fock formalism. A new method for reaching various stationary Hartree-Fock points, not accessible by the usual adiabatic constrained Hartree-Fock method, is proposed.

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The ultimate test of the theories describing the nuclear large amplitude collective motion is provided by experimental data. Of particular interest are the measurements of coexisting nuclear states built upon configurations with very different intrinsic properties. It has been early recognized that various nuclear collective modes and associated deformations could be attributed to specific symmetries of the intrinsic Hamiltonian [1]. The most common are the isoscalar and isovector shape deformations, and there are many spectacular examples of shape coexistence [2,3]: deformed rotational-like structures in spherical nuclei, superdeformed bands and fission isomers, and prolate and oblate states coexisting in the same nucleus. However, the concept of deformation is more general and is not solely related to shape degrees of freedom. For example, for strong pairing forces, there appear deformations that can be associated with static pairing gaps defining the orientation of a nucleus in the gauge space. Interesting pairing deformations are expected in $N \sim Z$ nuclei, where strong neutron-proton correlations are likely to produce a static moment that will lead to a spontaneous breaking of isospin (The elementary excitations of such systems are represented by quasi-particles which are mixtures of protons and neutrons.) In all the cases mentioned above, the underlying physics is governed by a coexistence of several stable mean fields with different deformations in one nucleus.

The origin of the coexistence phenomenon can be explained in terms of several local minima in the potential energy surface (PES) in the time-dependent Hartree-Fock (TDHF) manifold. Introducing more than two local minima, usually not orthogonal with one another, requires the full analysis of the gauge structure of the TDHF manifold [4]. In this paper, however, we only concentrate on the generic features of the minimum points in the TDHF manifold. For simplicity, the discussion is focused on the particle-hole aspects of the problem; the effects due to pairing interaction will be discussed in subsequent publications.

The constrained (C-)HF method (or its approximation through the Nilsson-Strutinsky method) has proved to be quite successful in explaining vast amounts of experimental data. However, in practical CHF applications, usually only the the lowest-energy solution under a given constraining condition is considered (adiabatic assumption). A corresponding set of single-particle states in the intrinsic system, defined by the adiabatic (A-)CHF solution, satisfies a non-crossing rule. On the other hand, in both the nuclear structure and nuclear reaction theories, there have been proposed various diabatic prescriptions based on the concept of intrinsic (self-consistent) quantum numbers. The basic building blocks in such approaches are diabatic single-particle orbits defining the intrinsic single-particle configuration. Since the intrinsic quantum numbers are (nearly) conserved, the corresponding orbitals cross sharply. (For a recent review of diabatic approaches, see, e.g., ref. [5] and references quoted therein.) So far, however, no solid theoretical justification of the diabatic recipe has been given. In this Letter, a new method, the so-called configuration-constrained Hartree-Fock (CCHF) method, is formulated. Based on the properties of the CHF solution near the PES saddle points, the CCHF method makes it possible to reach many (stable and unstable) stationary HF points in the TDHF manifold.

The features of adiabatic and diabatic single-particle states should be studied by analyzing the structure of the PES in the TDHF manifold; i.e., using a complete set of canonical variables rather than a limited number of constraining coordinates. In the following, the essential points of the CCHF method are illustrated using a simple soluble $SU(3)$ model [6] which, due to a small number of canonical variables, allows for a transparent presentation

of results. The SU(3) Hamiltonian consists of three N -fold degenerate levels with energies $\epsilon_0 < \epsilon_1 < \epsilon_2$ and a two-body residual interaction:

$$\begin{aligned}\hat{H} &= \hat{H}_0 + \hat{H}_V + \hat{H}_Y, \\ \hat{H}_0 &= \epsilon_0 \hat{K}_{00} + \epsilon_1 \hat{K}_{11} + \epsilon_2 \hat{K}_{22}, \\ \hat{H}_V &= \frac{V_1}{2} (\hat{K}_{10} \hat{K}_{10} + h.c.) + \frac{V_2}{2} (\hat{K}_{20} \hat{K}_{20} + h.c.), \\ \hat{H}_Y &= V_3 (\hat{K}_{10} (\hat{K}_{11} + \hat{K}_{22}) + h.c.) + V_4 (\hat{K}_{10} (\hat{K}_{12} + \hat{K}_{21}) + h.c.) + \\ &\quad V_5 (\hat{K}_{20} (\hat{K}_{11} + \hat{K}_{22}) + h.c.) + V_6 (\hat{K}_{20} (\hat{K}_{12} + \hat{K}_{21}) + h.c.),\end{aligned}\quad (1)$$

where the particle-hole operator $\hat{K}_{ij}$ is defined as

$$\hat{K}_{ij} = \sum_{m=1}^N \hat{c}_{im}^\dagger \hat{c}_{jm}. \quad (2)$$

Hereafter, we consider a system with an even number of particles, N . The Hamiltonian (1) has more than two non-trivial HF points. Recently, a modified version of this Hamiltonian was discussed in a slightly different context in Refs. [7-9].

For the constraining operator $\hat{Q}$, we took the most general Hermitian one-body operator:

$$\begin{aligned}\hat{Q} &= Q_{1x}(\hat{K}_{10} + \hat{K}_{01}) + Q_{1y}(\hat{K}_{20} + \hat{K}_{02}) + Q_{2x}\hat{K}_{11} + Q_{2y}\hat{K}_{22} \\ &\quad + Q_3\hat{K}_{00} + Q_4(\hat{K}_{21} + \hat{K}_{12}).\end{aligned}\quad (3)$$

The general TDHF state $|\phi\rangle$ is expressed as

$$|\phi\rangle = e^{\hat{F}}|\phi_0\rangle, \quad \hat{F} = \sum_{i=1}^2 \{f_i \hat{K}_{i0} + h.c.\}, \quad (4)$$

where the HF state

$$|\phi_0\rangle = \prod_{m=1}^N \hat{c}_{0m}^\dagger |0\rangle, \quad (\hat{c}_{im}|0\rangle = 0), \quad (5)$$

satisfies $\delta\langle\phi_0|\hat{H}|\phi_0\rangle = 0$. The TDHF equations can be written as

$$i\hbar\dot{\hat{C}}_j = \partial H / \partial \hat{C}_j^*, \text{ and c.c.; } j = 1 \text{ and } 2, \quad H = \langle\phi|\hat{H}|\phi\rangle, \quad (6)$$

where the complete set of canonical variables $\{C_i, C_i^*\}$ is obtained from the particle-hole amplitudes (f_i, f_i^*) through the variable transformation

$$C_i = \sqrt{N} f_i \frac{\sin \sqrt{\sum_j f_j^* f_j}}{\sqrt{\sum_j f_j^* f_j}} \text{ and } (i = 1 \text{ and } 2). \quad (7)$$

In the case of the considered SU(3) model, it is convenient to introduce the canonical coordinates x, y and the corresponding momenta:

$$\begin{aligned}x &= (C_1 + C_1^*)/\sqrt{2}, \quad p_x = i(C_1 - C_1^*)/\sqrt{2}, \\ y &= (C_2 + C_2^*)/\sqrt{2}, \quad p_y = i(C_2 - C_2^*)/\sqrt{2}.\end{aligned}\quad (8)$$

(Hereafter, the coordinate space $\{x, y\}$ is called the TDHF coordinate space.) Equations (6)-(8) demonstrate that the TDHF manifold $\{C, C^*\}$ has the same symplectic structure as the classical phase space. The aim of the general theory of nonlinear dynamics [10] has been to explore the complex structure of the classical phase space which is obtained by solving the equations of motion (6) with various initial conditions. However, in order to study the extremely rich structure of the TDHF manifold, the local minimum and maximum points of the PES in the TDHF manifold have to be found. For this aim, one usually employs the CHF method with a suitably chosen set of constraining operators [11].

It often happens in the realistic CHF calculation that an appreciable change in the occupation probability of very few single-particle orbits takes place in a tiny region of the constraining variables. In other words, a strong mixing among many single-particle orbits may be induced by many sequential local rearrangements that involve only a few single-particle states. The simple model Hamiltonian (1) is expected to simulate such a situation.

In order to calculate the PES for the Hamiltonian (1), we employ the matrix representation of the one-body operators expressed through the canonical coordinates x and y [defined in Eq. (8)]. The result is

$$\begin{aligned}\hat{F} &\Rightarrow F = \begin{pmatrix} 0 & 0 & f_2 \\ 0 & 0 & f_1 \\ -f_2 & -f_1 & 0 \end{pmatrix}, \\ e^{\hat{F}} &\Rightarrow e^F = \begin{pmatrix} 1 - \alpha y^2 & -\alpha xy & \beta y \\ -\alpha xy & 1 - \alpha x^2 & \beta x \\ -\beta y & -\beta x & 2\beta \gamma \end{pmatrix},\end{aligned}\quad (9)$$

where

$$\alpha = [2N + \sqrt{2N(2N - x^2 - y^2)}]^{-1}, \quad \beta = \frac{1}{\sqrt{2N}}, \quad \text{and } \gamma = \sqrt{\frac{1}{2} \left(N - \frac{x^2 + y^2}{2} \right)}. \quad (10)$$

In terms of the canonical coordinates, the matrix representation of the density matrix, $\hat{\rho}$ ($\rho_{ij} \equiv \langle\phi|\hat{K}_{ji}|\phi\rangle$), and the CHF one-body Hamiltonian, $\{\hat{H} - \lambda\hat{Q}\}_{\text{one-body}}$, are given by

$$\rho = \frac{1}{2} \begin{pmatrix} y^2 & xy & \gamma y \\ xy & x^2 & \gamma x \\ \gamma y & \gamma x & 4\gamma^2 \end{pmatrix}, \quad (11)$$

and

$$\mathcal{H} = e^{-F} h e^F, \quad h_{ij} = \frac{\partial(V - \lambda Q)}{\partial \rho_{ji}}, \quad (i, j = 0, 1, \text{ and } 2), \quad (12)$$

where

$$V(x, y) = \langle\phi|\hat{H}|\phi\rangle \quad \text{and} \quad Q(x, y) = \langle\phi|\hat{Q}|\phi\rangle \quad (13)$$

define the potential energy surface and Q -surface in the coordinate space, respectively. The CHF equations are:

$$\delta\langle\phi|\hat{H} - \lambda\hat{Q}|\phi\rangle = \delta(V(x, y) - \lambda Q(x, y)) = 0, \quad (14)$$

$$\langle\phi|\hat{Q}|\phi\rangle = Q(x, y) = q. \quad (15)$$

In the canonical representation, Eq. (14) can be expressed as

$$\frac{\partial V}{\partial x} = \lambda \frac{\partial Q}{\partial x}, \quad \frac{\partial V}{\partial y} = \lambda \frac{\partial Q}{\partial y}, \quad (16)$$

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

It is desirable to analyze the structure of the CHF solutions within the TDHF coordinate space. From Eq. (16), by eliminating the Lagrange multiplier λ , one obtains:

$$\frac{\partial V}{\partial y} \frac{\partial Q}{\partial x} - \frac{\partial V}{\partial x} \frac{\partial Q}{\partial y} = 0. \quad (17)$$

The above relation defines continuous (differentiable) lines in the TDHF coordinate space. The Lagrange multiplier λ is then computed using Eq. (16) at each point on the resultant lines. By means of the second CHF equation (15), one obtains the relation $\{x, y\} \rightarrow \{q\}$; i.e., the transformation from $\{x, y\}$ to the constraining coordinate space $\{q\}$.

In our calculations, we employed the following set of parameters of the Hamiltonian (1): $N = 4, e_0 = 0, e_1 = 16.4, e_2 = 18, V_1 = V_2 = -16/3, V_3 = -4/15, V_4 = -2/15, V_5 = 0, V_6 = -8/3$. This choice of parameters guarantees that the PES of the system in the coordinate space has three stable HF points (denoted by $|\phi_0\rangle, |\phi_1\rangle$, and $|\phi_2\rangle$ in Fig. 1a) and two unstable HF-points (saddle points, denoted by $|\phi_3\rangle$ and $|\phi_4\rangle$ in Fig. 1a). In a region near $x^2 + y^2 = 2N$ (not shown in Fig. 1a), there are three additional unstable HF points (one saddle and two maxima); they are irrelevant to the following discussion. It is to be noted that the PES does not have any apparent symmetry in the coordinate space; in particular, the minima at $|\phi_1\rangle$ and $|\phi_2\rangle$ are not degenerate.

The parameters of the constraining operator (3) are: $Q_{1x} = 1, Q_{1y} = 1/5, Q_{2x} = Q_{2y} = 2$, and $Q_3 = Q_4 = 0$. The contour map of $Q(x, y)$ is displayed in Fig. 1b. The above choice of $\hat{Q}$ guarantees that the solution of Eq. (17) has two branches in the $\{x, y\}$ space. In Fig. 1a, these two solutions (denoted by A and B) are superimposed on the PES. The two branches do not cross each other; every HF point rests on one of these lines. It is to be noted that $\hat{Q}$ represents a general one-body operator; its physical sense is hidden in the values of Q_i 's. In practice, the choice is rather arbitrary and strongly depends on the physics problem in question. In other words, the operator $\hat{Q}$ does not represent physical reality (i.e., the motion of the system in the full $\{x, y\}$ -space) but rather a certain projection of the motion determined by the structure of $Q(x, y)$ in the coordinate space. Moreover, in practical microscopic calculations, the dimension of the constraining coordinate space is very small as compared to the dimension of the coordinate space. Our simple model has two coordinates $\{x, y\}$. Consequently, only one constraint q has been chosen.

By using the mapping $\{x, y\} \rightarrow \{q\}$, the potential energy curves corresponding to trajectories A and B of Fig. 1 are constructed; they are displayed in Fig. 2. As is seen in Figs. 1 and 2, in certain regions of $\{q\}$ the CHF equations have more than one solution. To

avoid ambiguity, one may choose the most energetically favorable branch by applying the adiabatic approximation. This gives an adiabatic PES in $\{q\}$, $V_{\text{adia.}}(q)$, indicated by a thick dashed line in Fig. 2. The adiabatic surface contains only partial information about the full CHF solution. In particular, the information about the second stable HF point $|\phi_2\rangle$ is lost. It should also be emphasized that there is *no dynamical reason* to connect a set of the most energetically favorable states.

Let us consider how to reach the HF state $|\phi_2\rangle$ situated on line B starting from line A. According to the diabatic recipe, the diabatic CHF solution can be obtained by freezing the occupation probabilities of the mean-field Hamiltonian $\{\hat{H} - \lambda\hat{Q}\}_{\text{one-body}}$. In practice, it is achieved by removing the virtual interaction between the single-particle levels. In the following, we examine this procedure from what is happening in the TDHF manifold.

In order to make the presentation more transparent, the part of the PES near the saddle points is shown in Fig. 3. Let us begin by selecting a point (x_0, y_0) on line A near the saddle point. In our model, the particle number in orbit 1 stays constant along the vertical line (parallel to ordinates) with $x = x_0$. [The particle number in orbit 2 remains constant along the horizontal line (parallel to abscissas) with $y = y_0$. Note also that the single-particle orbits specifying the intrinsic configuration are not necessarily chosen at $|\phi_0\rangle$.] Let us impose the diabatic constraint by freezing the occupation of orbit 1. The solution of the first CHF equation (16) along the line $x = x_0$,

$$\left(\frac{\partial V}{\partial x} - \lambda_x \frac{\partial Q}{\partial x}\right)\Big|_{x=x_0} = 0, \quad (18)$$

defines the Lagrange multiplier $\lambda_x(x_0, y)$. Here it should be noted that the condition (18) is equivalent to $\mathcal{H}_{10}(x_0, y) = 0$. Of course, since the second equation (16) is violated, the condition $\mathcal{H}_{20}(x_0, y) = 0$ is not met. The second equation (16) along the $x = x_0$ line,

$$\left(\frac{\partial V}{\partial y} - \lambda_y \frac{\partial Q}{\partial y}\right)\Big|_{x=x_0} = 0, \quad (19)$$

[equivalent to $\mathcal{H}_{20}(x_0, y) = 0$] defines the Lagrange multiplier $\lambda_y(x_0, y)$. At points α and β in Fig. 3, there holds a relation

$$\lambda_x(x_0, y) = \lambda_y(x_0, y). \quad (20)$$

Equations (18)-(20) constitute the basic equations of the CCHF method which defines a way of reaching line B by starting from a certain point on line A near the saddle point. After reaching point α , where the relation $\mathcal{H}_{10}(x_0, y) = \mathcal{H}_{20}(x_0, y) = 0$ is satisfied, one can switch back to the usual CHF method to find another HF point $|\phi_2\rangle$ on line B. Figure 4 displays the calculated values of $\lambda_x(x_0, y)$ and $\lambda_y(x_0, y)$.

Along the vertical line $x = x_0$, the one-body Hamiltonian $\{\hat{H} - \lambda\hat{Q}\}_{\text{one-body}}$ with $\lambda = \lambda_x(x_0, y)$ does not define the single-particle states because $\mathcal{H}_{20}(x_0, y) \neq 0$ except for the intersection points. There are two ways of defining the single-particle states between points (x_0, y_0) and α (or β). Namely, one can either (i) use $\lambda_x(x_0, y)$ and eliminate $\mathcal{H}_{20}(x_0, y)$ by regarding it as a virtual interaction, or (ii) use $\lambda_y(x_0, y)$ and eliminate $\mathcal{H}_{10}(x_0, y)$. This ambiguity does not cause any trouble when one wants to reach the intersection point on the way to the HF point $|\phi_2\rangle$. Elimination of the virtual interaction thus effectively induces

a subtle change in the PES, so as to connect line A with line B through the vertical line indicated in Fig. 3. Since the diabatic recipe in the Nilsson-Strutinsky method is based on an effective one-body Hamiltonian $\{\hat{H} - \lambda\hat{Q}\}_{\text{one-body}}$, various properties of the PES can be specified by only defining appropriate single-particle states, like the diabatic single-particle states.

The CCHF method developed in this study can be a useful tool when applied to systems with weak particle-particle interaction (pairing). It is known, however, that in most cases the pairing interaction does play an important role in the process of mixing coexisting HF vacua [12–17]. The generalization of the CCHF method to the case of pairing will be discussed in subsequent publications.

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FIGURES

FIG. 1. Contour map of (a) PES $V(x, y)$, and (b) the constraining operator $Q(x, y)$. Continuous lines denoted by A and B are solutions of the CHF equation (17) in the TDHF coordinate space $\{x, y\}$.

FIG. 2. Potential energy curves along the branches A and B of Fig. 1 versus $\langle \dot{Q} \rangle$. They are calculated by using a set of points indicated in Fig. 1b. The dashed and dotted-dash curves correspond to the upper and lower branches of B, whereas the full curves to A. The curvature tensor (stability matrix) [11] for the upper branch of B is negative. The adiabatic potential energy, $V_{\text{adia.}}$, is indicated by a thick dashed line.

FIG. 3. Contour map of potential energy surface near the saddle points. Along the vertical line $x = x_0$, the particle number in orbit 1 is kept constant. Intersection points with line B are denoted by α and β .

FIG. 4. Lagrange multipliers $\lambda_x(x_0, y)$ and $\lambda_y(x_0, y)$ along the line $x = x_0$ of Fig. 3.

Fig.1 (a)

Fig.1 (b)

Fig.2

Fig.3

Fig.4