

Adiabatic time-dependent Hartree-Fock theory with the Skyrme interaction

A. K. Mukherjee

Saha Institute of Nuclear Physics, Calcutta 700 009, India

(Received 5 February 1990)

A derivation for reducing the adiabatic time-dependent Hartree-Fock theory with the consistency condition to an efficacious form, in which the evolution of the single-particle states is given by a time-dependent Hartree-Fock-like equation while the consistency condition is given by a one-body equation, is discussed. The density-dependent Skyrme interaction is included in the derivation.

I. INTRODUCTION

The adiabatic time-dependent Hartree-Fock (ATDHF) theory for the microscopic description of the large-amplitude collective motions of nuclei, e.g., fission, fusion, etc., has been formulated by Villars,¹ by Baranger and Vénéroni,² and by Goeke and Reinhard.³ In Ref. 4, the formal identity of the approaches was established while arguing that, for consistent exploitation of the TDHF variation principle in the adiabatic limit, the second-order ATDHF equation, in conjunction with the zeroth- and first-order (Villars) equations, has to be taken into account. Nonuniqueness^{5,6} of Villars equations was lifted by imposing the consistency condition derived from the zeroth- and second-order equations via the elimination of the curvature term. Use of a formal but analytic operator algebra method then showed⁴ that the simultaneous fulfillment of Villars equations and the consistency condition results in a unique path following the bottom of the valley of the many-body potential-energy surface for any adiabatic process. The canonicity condition completes⁷ the above proof regarding the valley by determining the Lagrange multiplier.

Instead of including an outline of the ATDHF theory in the state-vector formalism,⁶ in Sec. II A, we give a short account of the theory in the density-matrix form for reasons to be understood in the course of this paper. The one-body form of the ATDHF equations given in Sec. II A is written, in Sec. II B, in the particle-hole (p - h) space which is defined as the representation² in which the time-even density matrix is diagonal. The Villars equations are combined to yield a TDHF-like equation for the evolution of the single-particle states with respect to the collective coordinate q . The consistency condition is reduced to a one-body form involving only the occupied (hole) single-particle states. The advantage of this reduction of the ATDHF equations is that they do not require the knowledge of the infinite number of unoccupied (particle) states and thus do not need to be simulated by the effect of continuum, as has been done in random-phase approximation (RPA) calculations.⁸

In recent years, the mean-field description of nuclear dynamics was used⁹⁻²⁰ by several workers in describing

various nuclear processes. While in Refs. 9-13, the ATDHF formalism was used, in Refs. 14-16 and 17-20, the TDHF and constrained HF+BCS formalism was invoked. In the context of the ATDHF formalism, a truncated version of the THDF-like evolution equation derived here was used by Goeke *et al.*⁹⁻¹² but they have not used the consistency condition which should be fulfilled by the single-particle states during their evolution according to the TDHF-like equation in order that the extracted solution is the optimal valley path.

In the mean-field approximation, the effective two-body interaction used is predominantly density dependent. The Skyrme interaction^{21,22} was used in the HF calculations²³ as well as in the TDHF calculations.¹⁴ In the TDHF theory, the Skyrme interaction is included formally by Engel *et al.*²⁴ In Sec. III we give an account of the coordinate representation of the ATDHF theory with Skyrme interaction.

Several local densities can be constructed from the one-body density matrix, the later being a solution to the TDHF equation and having no specific behavior under time reversal. A set of these local densities, e.g., particle density, kinetic-energy density, spin current tensor, is even under time reversal while the other set, e.g., spin density, momentum density, kinetic-energy density (vector part), is odd under time reversal. Under the adiabatic expansion of the (time-mixed) density matrix of the TDHF equation, it has been shown in Sec. III A that, while the time-even local densities are expanded in even powers of the adiabaticity parameter p , the time-odd local densities are expanded in odd powers of p . In Sec. III B, using these expansions of the local densities, the collective Hamiltonian is obtained in the classical form in which the collective mass and the collective potential are given as algebraic functions of the local densities. In Sec. III C, following Engel *et al.*, the ATDHF equations with the Skyrme interaction are obtained in the same form of a TDHF-like evolution equation and a one-body consistency condition; only the HF Hamiltonian in different orders of p is given as a function of the local densities.

Section V contains the conclusions of the present work. A preliminary version of a part of the present work appeared in a conference report.²⁵

II. ATDHF THEORY WITH THE CONSISTENCY CONDITION

A. One-body form of the ATDHF equations

The time-dependent Hartree-Fock equation in the density-matrix form is given by¹⁴

$$i\dot{\rho} = [h, \rho], \quad (1)$$

where the one-body TDHF Hamiltonian h is given by

$$h = t + \text{Tr}\bar{v}\rho. \quad (2)$$

Here t is the kinetic-energy operator and v is the two-body interaction potential. The matrix elements of the trace are defined as

$$\langle a | \text{Tr}\bar{v}\rho | b \rangle = \sum_{\alpha\beta} (a\alpha | v | b\beta) \langle \beta | \rho | \alpha \rangle. \quad (3)$$

Here $|a\rangle$, $|b\rangle$, $|\alpha\rangle$, $|\beta\rangle$ etc., are the single-particle states and the parenthesis matrix element of the two-body interaction potential v stands for the usual direct minus exchange matrix element.

It is well known^{2,24} that the density matrix ρ appearing in the TDHF equation (1) does not have any specific behavior under time reversal. $\rho(t)$ contains both time-even and time-odd components. In the adiabatic approximation, such a (time-mixed) density matrix is parametrized as¹⁻⁴

$$\rho(t) = \rho(p, q) = \exp(-ip\hat{q})\rho_0(q)\exp(ip\hat{q}). \quad (4)$$

Here $\rho_0(q)$ is the time-even density matrix derived from the time-even Slater determinant $\Phi(q)$, which is parametrized in terms of the collective coordinate q and thus satisfies the idempotent condition

$$\rho_0^2 = \rho_0. \quad (5)$$

In Eq. (4), p is the small adiabaticity parameter and \hat{q} is assumed to be a one-body time-even Hermitian (p - h) operator. The coordinate q and the adiabaticity parameter p , the later playing the role of conjugate momentum, should satisfy Hamilton's equations

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p}, \quad \dot{p} = -\frac{\partial \mathcal{H}}{\partial q}, \quad (6)$$

where the collective Hamiltonian \mathcal{H} is given by

$$\mathcal{H}(p, q) = \frac{p^2}{2m(q)} + V(q). \quad (7)$$

Here the collective mass $m(q)$ and the collective potential $V(q)$ are given by

$$m^{-1}(q) = \text{Tr}h_0[[\hat{q}, \rho_0], \hat{q}] + \text{Tr}\text{Tr}[\hat{q}, \rho_0]\bar{v}[\hat{q}, \rho_0], \quad (8a)$$

$$V(q) = \text{Tr}t\rho_0 + \frac{1}{2}\text{Tr}\text{Tr}\rho_0\bar{v}\rho_0, \quad (8b)$$

where

$$h_0 = t + \text{Tr}\bar{v}\rho_0. \quad (9a)$$

Hamilton's equation (6) follows from the TDHF variation principle provided the following normalization require-

ment, usually called the canonicity condition, is fulfilled:¹⁻⁴

$$\text{Tr}[\hat{q}, -i\hat{p}]\rho_0 = 1. \quad (10)$$

Here \hat{p} is a one-body time-odd (p - h) operator defined through

$$\frac{\partial \rho_0}{\partial q} = [-i\hat{p}, \rho_0]. \quad (11)$$

Expanding the TDHF equation (1) under the adiabatic decomposition (4) in powers of p gives, respectively, the zeroth-, first-, and second-order ATDHF equations in the density-matrix form

$$[O_0, \rho_0] = 0, \quad (12)$$

$$[O_1, \rho_0] = 0, \quad (13)$$

$$[O_2, \rho_0] = 0, \quad (14)$$

where the one-body operators O_0 , O_1 , and O_2 are given by

$$O_0 = h_0 - \lambda\hat{q}, \quad (15a)$$

$$O_1 = [h_0, \lambda\hat{q}] + \bar{h}_1 + i\frac{\lambda}{m}\hat{p}, \quad (15b)$$

$$O_2 = -\frac{1}{2}([[h_0, \lambda\hat{q}], \lambda\hat{q}] + 2[\bar{h}_1, \lambda\hat{q}] + \bar{h}_2) + \frac{\lambda^2}{m}\frac{d\hat{q}}{dq} - \frac{1}{2}\lambda^2\frac{dm^{-1}}{dq}\hat{q}. \quad (15c)$$

The TDHF Hamiltonians h to different orders of p are given by

$$h_0 = t + \text{Tr}\bar{v}\rho_0, \quad (9a)$$

$$\bar{h}_1 = \frac{\lambda}{p}h_1 = \text{Tr}\bar{v}[\lambda\hat{q}, \rho_0], \quad (9b)$$

$$\bar{h}_2 = -\frac{\lambda^2}{2p^2}h_2 = \text{Tr}\bar{v}[\lambda\hat{q}, [\lambda\hat{q}, \rho_0]], \quad (9c)$$

where

$$\lambda = \frac{dV}{dq}. \quad (16)$$

All these equations given above in the density-matrix form are the same as those in the state-vector form derived earlier.^{1-4,6} The identity of the ATDHF equations (12)–(14) and those in the state-vector form can easily be established²⁵ from well-known results²⁶ of many-body matrix elements between determinantal states.

In a manner similar to that followed in Ref. 4, the consistency condition is obtained by eliminating the curvature term $d\hat{q}/dq$ from Eq. (14) and the equation obtained by differentiating Eq. (12) with respect to q in the form

$$[O_c, \rho_0] = 0, \quad (17)$$

where

$$O_c = -\frac{1}{2}([h_0, \lambda \hat{q}], \lambda \hat{q}) + 2[\bar{h}_1, \lambda \hat{q}] + \bar{h}_2) \\ + \frac{\lambda}{m} \left[[h_0, -i\hat{p}] + \frac{dh_0}{dq} \right] - \lambda \omega_0(q) \hat{q}, \quad (18)$$

$$\omega_0(q) = \frac{1}{2\lambda} \frac{d}{dq} (\lambda^2/m). \quad (19)$$

B. Representation in p - h space

The ATDHF equations (12), (13), and (17) should be solved² in a representation in which the time-even density matrix $\rho_0(q)$ is diagonal. In this section we cast the Villars equations (12) and (13) and the consistency condition (17) in the said representation.

Equations (12) and (13) represent²⁵ the fact that the p - h and h - p matrix elements of the operators $\lambda \hat{q}$ and $-i(\lambda/m)\hat{p}$ are equal to those of the operators h_0 and $\hat{e} = [h_0, \lambda \hat{q}] + \bar{h}_1$, respectively.

Since, by definition, the p - p and h - h matrix elements of \hat{q} and \hat{p} vanish, we have

$$\lambda \hat{q} = (1 - \rho_0) h_0 \rho_0 + \rho_0 h_0 (1 - \rho_0), \quad (20)$$

$$-i\hat{p} = c(q) [\rho_0 \hat{e}(q) (1 - \rho_0) + (1 - \rho_0) \hat{e}(q) \rho_0]. \quad (21)$$

In deriving Eq. (21), Eq. (20) has been used. Here,

$$\hat{e}(q) = [h_0 (1 - 2\rho_0) h_0, \rho_0] + \bar{h}_1, \quad (22)$$

$$\bar{h}_1 = \text{Tr} \bar{v} [h_0, \rho_0], \quad (23)$$

$$c(q) = m(q) / \lambda(q). \quad (24)$$

The evolution of the time-even density matrix ρ_0 is thus given by Eq. (11) where the evolution operator $-i\hat{p}$ is given in Eq. (21) in terms of known quantities.

The evolution of the occupied single-particle states $|\phi_h(q)\rangle$ are therefore given by

$$\frac{\partial}{\partial q} |\phi_h(q)\rangle = c(q) (1 - \rho_0) \hat{e}(q) |\phi_h(q)\rangle. \quad (25)$$

The similarity of the ATDHF evolution equation (25) or (11) with the TDHF equation (1) is readily seen; only the TDHF evolution operator \hat{h} should now be replaced by $-i\hat{p}$ which is given in Eq. (21).

The consistency condition (17), after the substitution of the operators $\lambda \hat{q}$ and $-i\hat{p}$ from Eqs. (20) and (21), respectively, reduces to the one-body form

$$[R, \rho_0] = 0, \quad (26)$$

where the consistency operator R is given by

$$R = [h_0, \hat{e}] + \bar{h}_c - \omega_0(q) h_0. \quad (27)$$

Here,

$$\bar{h}_c = \bar{h}_q - \frac{1}{2} \bar{h}_2, \quad (28a)$$

$$\bar{h}_q = \text{Tr} \bar{v} [\hat{e}, \rho_0], \quad (28b)$$

$$\bar{h}_2 = \text{Tr} \bar{v} [(1 - \rho_0) h_0 \rho_0 + \rho_0 h_0 (1 - \rho_0), [h_0, \rho_0]]. \quad (28c)$$

The p - h matrix elements of Eq. (26) give

$$(1 - \rho_0) R |\phi_h(q)\rangle = 0. \quad (29)$$

Note from Eqs. (21) and (27) that the evolution operator $-i\hat{p}$ and the consistency operator R do not require the knowledge of an infinite number of particle states.

We thus have a representation of the ATDHF equations in which the occupied single-particle states evolve in accordance with the TDHF-like equation (25) so that the numerical methods¹⁴ of solving the TDHF equation can be used here with minor modifications. Further, in order to obtain the valley solution from the infinite number of solutions of the Villars equations (12) and (13) or, equivalently, Eq. (25), we are required to fulfill a one-body consistency condition (29).

The set of single-particle states $|\phi_h(q_0 + \delta q)\rangle$ at $q = q_0 + \delta q$ in terms of the initial state $|\phi_h(q_0)\rangle$ at $q = q_0$, following Eq. (25), is given by

$$|\phi_h(q_0 + \delta q)\rangle = \exp[-i\delta q \hat{p}(q_0)] |\phi_h(q_0)\rangle. \quad (30)$$

We note here that the prescription⁹⁻¹²

$$|\phi_h^0(q_0 + \delta q)\rangle = [1 - i\delta q \hat{p}(q_0)] |\phi_h(q_0)\rangle \quad (30a)$$

is a first-order truncation of Eq. (30). In contrast to Eq. (30) or (25), the scalar product of the single-particle states during the evolution with q in accordance with Eq. (30a) is not preserved. Thus, initializing with an orthonormal set $|\phi_h(q_0)\rangle$, the evolved set $|\phi_h^0(q_0 + \delta q)\rangle$ does not remain orthogonal. Using the prescription (30a), Goeke *et al.*⁹⁻¹² have orthogonalized the evolved set $|\phi_h^0(q_0 + \delta q)\rangle$ to obtain a new set $|\phi_h^{0'}(q_0 + \delta q)\rangle$. With the use of the new set $|\phi_h^{0'}(q_0 + \delta q)\rangle$, the collective mass and collective potential is extracted which, in turn, gives the physical observables like fusion cross section, etc., in the Wentzel-Kramers-Brillouin (WKKB) approximation. In the context of the Schmidt orthogonalization procedure,²⁷ we note here that, from n linearly independent vectors, one can construct at least n sets of possible orthonormalized vectors depending on the choice of the vector (from the linearized set) used to initialize the orthogonalization procedure. This fact may raise the confusion that the ATDHF solutions, i.e., $\phi_h^{0'}$ obtained in Refs. 9-12, are nonunique and, hence, the results obtained in these works are ambiguous. However, rotation of hole states among themselves without invoking the particle states leaves the density-matrix invariant. Since, in $m(q)$ and $V(q)$, the single-particle states enter only through the convolution of relevant operators with the density matrix, the outcome of the theory is the same for all such sets of states $\phi_h^{0'}$ that are related to each other through rotations among themselves.

III. COORDINATE REPRESENTATION WITH SKYRME INTERACTION

A. Adiabatic expansions of the local densities

The Slater determinantal state $|\Psi(t)\rangle$ comprised of the single-particle states $|\psi_h(t)\rangle$, which are the solutions to the TDHF equation (1), does not have any specific behavior under time reversal. The properties of the (time-mixed) density matrix $\rho(t)$ of such single-particle states

$|\psi_h(t)\rangle$ have been studied by Engel *et al.*²⁴

Let us define the scalar part $\rho(r, r')$ and the vector part $s(r, r')$,

$$\rho(r\sigma, r'\sigma') = \frac{1}{2}[\rho(r, r') + \delta_{\sigma\sigma'} + \langle \sigma | \sigma | \sigma' \rangle \cdot s(r, r')] , \quad (31)$$

where

$$\rho(r, r') = \sum_{\sigma} \rho(r\sigma, r'\sigma) , \quad (32a)$$

$$s(r, r') = \sum_{\sigma, \sigma'} \rho(r\sigma, r'\sigma') \langle \sigma' | \sigma | \sigma \rangle , \quad (32b)$$

and $\rho(r\sigma, r'\sigma')$ is the coordinate representation of the diagonal part in the isospin space of ρ . These scalar $\rho(r, r')$ and vector $s(r, r')$ parts have the time-reversal properties

$$\rho^T(r, r') = \rho(r', r) , \quad (33a)$$

$$s^T(r, r') = -s(r', r) . \quad (33b)$$

$\rho(r, r')$ and $s(r, r')$ can be used to define real local densities which have specific behavior under time reversal. They are the following:

(i) Particle density,

$$\rho(r) = \rho(r, r) . \quad (34a)$$

(ii) Kinetic-energy density,

$$\tau(r) = [\nabla \cdot \nabla' \rho(r, r')]_{r=r'} . \quad (34b)$$

(iii) Spin current tensor,

$$J_{\mu\nu}(r) = \frac{1}{2i} [(\nabla_{\mu} - \nabla'_{\mu}) s_{\nu}(r, r')]_{r=r'} . \quad (34c)$$

(iv) Spin density,

$$s(r) = s(r, r) . \quad (35a)$$

(v) Momentum density,

$$\mathbf{j}(r) = \frac{1}{2i} [(\nabla - \nabla') \rho(r, r')]_{r=r'} . \quad (35b)$$

(vi) Kinetic-energy density (vector part)

$$\mathbf{T}(r) = [\nabla \cdot \nabla' s(r, r')]_{r=r'} . \quad (35c)$$

Let us introduce the compact notation

$$\rho(r) = \begin{pmatrix} \rho(r) \\ \tau(r) \\ \mathbf{J}(r) \end{pmatrix} , \quad (36)$$

$$\mathbf{s}(r) = \begin{pmatrix} s(r) \\ \mathbf{j}(r) \\ \mathbf{T}(r) \end{pmatrix} . \quad (37)$$

It follows from Eqs. (33) that the local densities (36) are time even,

$$\rho^T(r) = \rho(r) , \quad (38a)$$

while the local densities (37) are time odd,

$$\mathbf{s}^T(r) = -\mathbf{s}(r) . \quad (38b)$$

The time-reversal properties (38) are obeyed by a general

(time-mixed) density matrix $\rho(t)$ and they follow from the construction (32).

In the adiabatic expansion of the (time-mixed) density matrix $\rho(t)$ we have

$$\begin{aligned} \rho(r\sigma, r'\sigma') &= \rho^{(0)}(r\sigma, r'\sigma') + p \bar{\rho}^{(1)}(r\sigma, r'\sigma') \\ &+ p^2 \bar{\rho}^{(2)}(r\sigma, r'\sigma') + \dots . \end{aligned} \quad (39)$$

Here $\rho^{(0)}(r\sigma, r'\sigma')$ is the coordinate representation of the time-even density matrix ρ_0 while $\bar{\rho}^{(1)}(r\sigma, r'\sigma')$ and $\bar{\rho}^{(2)}(r\sigma, r'\sigma')$ are those of the time-odd operator $\bar{\rho}_1 = [\lambda q, \rho_0]$ and the time-even operator $\bar{\rho}_2 = [[\lambda q, \rho_0], \rho_0]$, respectively.

The time-even density matrix ρ_0 , which, by Eq. (5), is derived from the time-even Slater determinant $|\Phi(q)\rangle$, can be used to define the local densities $\rho^{(0)}(r)$ and $\mathbf{s}^{(0)}(r)$ and it follows²⁸ from the construction (32) that

$$\mathbf{s}^{(0)}(r) = 0 . \quad (40)$$

However, since $\bar{\rho}_1$ and $\bar{\rho}_2$ are not density operators constructed from Slater determinants and thus do not satisfy the idempotency condition, analogous local densities cannot be defined. Nevertheless, since Eq. (32) is completely general, the coordinate representations $\bar{\rho}^{(1)}(r\sigma, r'\sigma')$ and $\bar{\rho}^{(2)}(r\sigma, r'\sigma')$ of $\bar{\rho}_1$ and $\bar{\rho}_2$ can be used to define the scalar and vector parts $\bar{\rho}^{(1)}(r, r')$, $s^{(1)}(r, r')$ and $\bar{\rho}^{(2)}(r, r')$, $s^{(2)}(r, r')$ which do not have the time-reversal properties (33). Now, using these scalar and vector parts, the local functions $\bar{\rho}^{(1)}(r)$, $\mathbf{s}^{(1)}(r)$ and $\rho^{(2)}(r)$, $\mathbf{s}^{(2)}(r)$ can be constructed but they are not densities and do not have the properties (38). However, in Appendix A we show,²⁸ by using time-reversal properties of $\bar{\rho}_1$ and $\bar{\rho}_2$, that

$$\bar{\rho}^{(1)}(r) = 0 , \quad (41a)$$

$$\mathbf{s}^{(2)}(r) = 0 . \quad (41b)$$

Utilizing Eqs. (40) and (41) in the adiabatic expansions of the local densities $\rho(r)$ and $\mathbf{s}(r)$, which are obtained from the expansion (39) of $\rho(r\sigma, r', \sigma')$, we have

$$\rho(r) = \rho^{(0)}(r) + p^2 \bar{\rho}^{(2)}(r) + \dots , \quad (42a)$$

$$\mathbf{s}(r) = p \mathbf{s}^{(1)}(r) + p^3 \mathbf{s}^{(3)}(r) + \dots . \quad (42b)$$

Thus, under the adiabatic expansion, the time-even local densities are expressed in even powers of p while the time-odd local densities are expressed in odd powers of p .

B. The collective Hamiltonian

The Skyrme interaction^{21,22} consists of a two-body term $v^{(2)}$ and a three-body term $v^{(3)}$, which, in the coordinate space, are

$$\begin{aligned} v^{(2)}(r_1, r_2) &= t_0(1 + x_0 P_{\sigma}) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ &+ \frac{1}{2} t_1 [\delta(\mathbf{r}_1 - \mathbf{r}_2) K^2 + K'^2 \delta(\mathbf{r}_1 - \mathbf{r}_2)] \\ &+ t_2 K' \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) K \\ &+ i V_{\text{SO}} (\sigma_1 + \sigma_2) K' \times \delta(\mathbf{r}_1 - \mathbf{r}_2) K , \end{aligned} \quad (43a)$$

$$v^{(3)}(r_1, r_2, r_3) = t_3 \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3) . \quad (43b)$$

Here $P_\sigma = \frac{1}{2}(1 + \sigma_1 \cdot \sigma_2)$ is the spin-exchange operator, $K = (1/2i)(\nabla_1 - \nabla_2)$ operates on the left, and $K' = -(1/2i)(\nabla_1 - \nabla_2)$ operates on the right.

The many-body Hamiltonian is then given by

$$H = \sum_i \left[-\frac{\hbar^2}{2m} \nabla_i^2 \right] + \sum_{i < j} v_{ij}^{(2)} + \sum_{i < j < k} v_{ijk}^{(3)}. \quad (44)$$

The expectation value of H in the TDHF Slater determinantal state $|\Psi\rangle$ has been derived in Ref. 24. It suffices to note here that one can write

$$E = \langle \Psi | H | \Psi \rangle = \int d^3r \mathcal{H}(r), \quad (45)$$

where the Hamiltonian density functional $\mathcal{H}(r)$ is given in Appendix B.

It is easily seen that, under the adiabatic expansions (42), the total energy reduces to the classical form²⁸

$$E = \mathcal{H}(p, q) = \frac{p^2}{2m(q)} + V(q), \quad (46)$$

where the collective mass $m(q)$ and collective potential $V(q)$ are given by

$$V(q) = \int d^3r \mathcal{V}(q, r), \quad (47a)$$

$$m(q) = \int d^3r \mathcal{M}(q, r). \quad (47b)$$

Here the potential density $\mathcal{V}(q, r)$ and the collective mass density $\mathcal{M}(q, r)$ are given in Appendix B.

C. The ATDHF equations

The variation of the binding energy E which, for the Skyrme interaction (43), can be written, following Ref. 24, as

$$\delta E = \sum_{\sigma q} \int d^3r \sum_k [\delta \psi_k^*(r, \sigma) h(r) \psi_k(r, \sigma) - \delta \psi_k(r, \sigma) h(r) \psi_k^*(r, \sigma)], \quad (48)$$

where $h(r)$ has been derived in Ref. 24 and, for completeness, the expression is repeated here in Appendix C.

The TDHF variation principle is given by^{14,29}

$$\int [\delta E - \delta \langle \Psi | i \partial / \partial t | \Psi \rangle] dt = 0. \quad (49)$$

Variation of the (time-mixed) single-particle states $\psi_k(r\sigma)$ with the adiabatic decomposition (4) gives²⁸ the ATDHF equations in the form of Eqs. (12)–(14) in which the coordinate representation of h_0 , \bar{h}_1 , and \bar{h}_2 are given in Appendix C. Note here that the result could also be obtained from the relation²⁹

$$\delta E = \text{Tr} h \rho \quad (50)$$

with the use of Eqs. (42).

IV. EVALUATION OF THE OPTIMAL PATH

The evaluation of the single-particle states $|\phi_h(q)\rangle$ is given by Eq. (25) in which the evolution operator $\hat{e}(q)$ is given in Eq. (22). The choice of q is expressed in terms of the measuring operator \hat{d} through¹

$$q = \text{Tr} \hat{d} \rho_0, \quad (51)$$

which gives

$$\text{Tr} [\hat{d}, -i\hat{p}] \rho_0 = 0. \quad (52)$$

Multiplying Eq. (52) by $c^{-1}(q)$, we have, using Eq. (21),

$$\frac{\lambda}{m} = c^{-1}(q) = \text{Tr} [\hat{d}, \hat{e}] \rho_0, \quad (53)$$

where the last equality is obtained by using the cyclic property of the trace. The choice of the parameter q expectedly determines the scaling of the single-particle states during their evolution with q . In addition, we have another normalization condition⁷ namely, the canonicity condition (10). Substituting \hat{p} and \hat{q} from Eqs. (20) and (21) in Eq. (10), we have

$$\frac{\lambda^2}{m} = \text{Tr} \rho_0 [\hat{e}(1 - \rho_0) h_0 - h_0 (1 - \rho_0) \hat{e}] \rho_0. \quad (54)$$

Combining Eqs. (53) and (54) we obtain the parameters λ and m separately while the potential $V(q)$ is obtained directly from Eq. (8b) or (B2a).

Though given a nonsingular initial condition, the TDHF-like equation can be solved in a manner similar to those used in TDHF calculations,¹⁴ the method of fulfillment of the consistency condition is not clear. A method to achieve the optimal solution of the Villars equations with the use of the consistency check derived in earlier sections and with the HF configuration as the initial state has recently been proposed in Ref. 30 where the method is successfully applied to explore the valley path in the soluble three-level model.

V. CONCLUSIONS

In this article, the ATDHF equations are reduced to a computationally amenable form in which the evolution of the single-particle states is given by a TDHF-like equation while the consistency condition is given by a one-body equation. The density-dependent two-body interaction is included in the derivation. Numerical calculation of fission event of ⁸Be following the method described in the text is in progress and will be reported elsewhere.

The author thanks Prof. M. K. Pal, Prof. K. Goeke, Prof. D. Pal, Prof. M. Vénéroni, Prof. H. Flocard, Prof. D. Vautherin, and Prof. G. DoDang for useful discussions and acknowledges the involvement of Prof. M. K. Pal in the early stage of the work.

APPENDIX A

The time-reversed local densities $\rho^T(r)$ and $\mathbf{s}^T(r)$ constructed from the time-reversed partner ρ^T of ρ satisfy Eqs. (38) and thus,

$$\begin{aligned} \rho^T(r) &= \rho(r) \\ &= \rho^{(0)}(r) + p \bar{\rho}^{(1)}(r) + p^2 \bar{\rho}^{(2)}(r) + \dots, \end{aligned} \quad (A1a)$$

$$\mathbf{s}^T(r) = -\mathbf{s}(r) = -p \mathbf{s}^{(1)}(r) - p^2 \mathbf{s}^{(2)}(r) - \dots, \quad (A1b)$$

where Eq. (40) has been used. Let $\rho^{T(1)}(r)$, $s^{T(1)}(r)$ and $\rho^{T(2)}(r)$, $s^{T(2)}(r)$ denote the local functions constructed from (32) with the time-reversed partners $\bar{\rho}_1^T$ and $\bar{\rho}_2^T$ of $\bar{\rho}_1$ and $\bar{\rho}_2$, respectively. The local densities $\rho^{T(r)}$ and $s^{T(r)}$ can also be expanded as

$$\rho^{T(r)} = \rho^{(0)}(r) + p\bar{\rho}^{T(1)}(r) + p^2\bar{\rho}^{T(2)}(r) + \dots, \quad (\text{A2a})$$

$$s^{T(r)} = ps^{T(1)}(r) + p^2s^{T(2)}(r) + \dots. \quad (\text{A2b})$$

Comparing Eqs. (A1) and (A2), we find that they are consistent if and only if

$$\bar{\rho}^{T(1)}(r) = \bar{\rho}^{(1)}(r), \quad s^{T(1)}(r) = -s^{(1)}(r), \quad (\text{A3a})$$

$$\bar{\rho}^{T(2)}(r) = \bar{\rho}^{(2)}(r), \quad s^{T(2)}(r) = -s^{(2)}(r). \quad (\text{A3b})$$

However, since $\bar{\rho}_1$ is time odd and $\bar{\rho}_2$ is time even, it follows from the definition (32) that

$$\rho^{T(1)}(r, r') = -\rho^{(1)}(r, r'), \quad (\text{A4a})$$

$$s^{T(1)}(r, r') = -s^{(1)}(r, r'),$$

$$\rho^{T(2)}(r, r') = \rho^{(2)}(r, r'), \quad (\text{A4b})$$

$$s^{T(2)}(r, r') = s^{(2)}(r, r').$$

The local functions constructed from $\bar{\rho}_1$ and $\bar{\rho}_2$ therefore have the time-reversal property

$$\bar{\rho}^{T(1)}(r) = -\bar{\rho}^{(1)}(r), \quad s^{T(1)}(r) = -s^{(1)}(r), \quad (\text{A5a})$$

$$\bar{\rho}^{T(2)}(r) = \bar{\rho}^{(2)}(r), \quad s^{T(2)}(r) = s^{(2)}(r). \quad (\text{A5b})$$

Comparing Eqs. (A3) and (A5), it follows that they are consistent if and only if

$$\bar{\rho}^{(1)}(r) = 0, \quad s^{(2)}(r) = 0. \quad (\text{A6})$$

APPENDIX B

As derived in Ref. 24, the Hamiltonian density functional $\mathcal{H}(r)$ introduced in Eq. (45) is given by

$$\begin{aligned} \mathcal{H}(r) = & \frac{\hbar^2}{2m} \tau + \frac{1}{2} t_0 \left[\left(1 + \frac{1}{2} x_0\right) \rho^2 - \left(x_0 + \frac{1}{2}\right) (\rho_p^2 + \rho_n^2) + \frac{1}{2} x_0 s^2 - \frac{1}{2} (s_n^2 + s_p^2) \right] \\ & + \frac{1}{4} (t_1 + t_2) (\rho \tau - j^2) + \frac{1}{8} (t_2 - t_1) \sum_q (\rho_q \tau_q - j_q^2 + s_q \cdot T_q - \vec{J}_q^2) + \frac{1}{16} (t_2 - 3t_1) \rho \nabla^2 \rho \\ & + \frac{1}{32} (t_2 + 3t_1) \sum_q (\rho_q \nabla^2 \rho_q + s_q \cdot \nabla^2 s_q) - \frac{1}{2} V_{\text{SO}} \sum_{qq'} (1 + \delta_{qq'}) (s_q \cdot \nabla \times j_{q'} + \rho_q \vec{\nabla} \cdot \vec{J}_{q'}) \\ & + \frac{1}{4} t_3 [\rho_p (\rho_n^2 - s_n^2) + \rho_n (\rho_p^2 - s_p^2)]. \end{aligned} \quad (\text{B1})$$

In the adiabatic approximation, the total energy reduces to the classical form (46) where the potential-energy density $\mathcal{V}(q, r)$ and the mass density $\mathcal{M}(q, r)$ introduced in Eqs. (47) are given by

$$\begin{aligned} \mathcal{V}(q, r) = & \frac{\hbar^2}{2m} \tau^{(0)} + \frac{1}{2} t_0 \left[\left(1 + \frac{1}{2} x_0\right) \rho^{(0)2} - \left(x_0 + \frac{1}{2}\right) (\rho_p^{(0)2} + \rho_n^{(0)2}) \right] + \frac{1}{4} (t_1 + t_2) \rho^{(0)} \tau^{(0)} \\ & + \frac{1}{16} (t_2 - 3t_1) \rho^{(0)} \nabla^2 \rho^{(0)} + \frac{1}{32} (t_2 + 3t_1) \sum_q \rho_q^{(0)} \nabla^2 \rho_q^{(0)} + \frac{1}{8} (t_2 - t_1) \sum_q (\rho_q^{(0)} \tau_q^{(0)} - \vec{J}_q^{(0)2}) \\ & - \frac{1}{2} V_{\text{SO}} \sum_{qq'} (1 + \delta_{qq'}) \rho_q^{(0)} \vec{\nabla} \cdot \vec{J}_{q'}^{(0)} + \frac{1}{4} t_3 (\rho_p^{(0)} \rho_n^{(0)2} + \rho_n^{(0)} \rho_p^{(0)2}), \end{aligned} \quad (\text{B2a})$$

$$\begin{aligned} \mathcal{M}(q, r) = & \frac{\hbar^2}{2m} \tau^{(2)} + \frac{1}{4} t_0 x_0 s^{(1)2} - \frac{1}{4} t_0 (s_p^{(1)2} + s_n^{(1)2}) - \frac{1}{4} (t_1 + t_2) j^{(1)2} + \frac{1}{32} (t_2 + 3t_1) \sum_q s_q^{(1)} \cdot \nabla^2 s_q^{(1)} \\ & + \frac{1}{8} (t_2 - t_1) \sum_q (s_q^{(1)} \cdot T_q^{(1)} - j_q^{(1)2}) - \frac{1}{2} V_{\text{SO}} \sum_{qq'} (1 + \delta_{qq'}) s_q^{(1)} \cdot \nabla \times j_{q'}^{(1)} - \frac{1}{4} t_3 (\rho_p^{(0)} s_n^{(1)2} + \rho_n^{(0)} s_p^{(1)2}) \\ & + \frac{1}{4} (t_1 + t_2) [\rho^{(0)} \tau^{(2)} + \rho^{(2)} \tau^{(0)}] + \frac{1}{16} (t_2 - 3t_1) (\rho^{(0)} \nabla^2 \rho^{(2)} + \rho^{(2)} \nabla^2 \rho^{(0)}) \\ & + \frac{1}{32} (t_2 + 3t_1) \sum_q (\rho_q^{(0)} \nabla^2 \rho_q^{(2)} + \rho_q^{(2)} \nabla^2 \rho_q^{(0)}) + \frac{1}{8} (t_2 - t_1) \sum_q (\rho_q^{(0)} \tau_q^{(2)} + \rho_q^{(2)} \tau_q^{(0)}) \\ & - \frac{1}{2} V_{\text{SO}} \sum_{qq'} (1 + \delta_{qq'}) (\rho_q^{(0)} \vec{\nabla} \cdot \vec{J}_{q'}^{(2)} + \rho_q^{(2)} \vec{\nabla} \cdot \vec{J}_{q'}^{(0)}) + \frac{1}{4} t_3 (\rho_p^{(2)} \rho_n^{(0)2} + \rho_n^{(2)} \rho_p^{(0)2}). \end{aligned} \quad (\text{B2b})$$

The variation of the energy functional $\mathcal{H}(r)$ gives δE in the form of Eq. (48) where the TDHF Hamiltonian h is given by²⁴

$$h_q(r) = -\nabla \frac{\hbar^2}{2m_q^*(r)} \nabla + U_q + \frac{1}{2i} (\vec{\nabla} \sigma \cdot \vec{B}_q + \vec{B}_q \cdot \vec{\nabla} \sigma) - \nabla \cdot (\sigma \cdot C_q) \nabla + \sigma \cdot \sum_q + \frac{1}{2i} (\nabla \cdot I_q + I_q \cdot \nabla), \quad (\text{C1})$$

where m_q^* , U_q , \vec{B}_q , C_q , \sum_q , and I_q are given in Ref. 24 [see Eqs. (B2)–(B7) of Ref. 24].

Substituting the expansion

$$\psi_k(r, \sigma) = \sum_{\sigma'} \int d^3r' \langle r\sigma | \exp(ip\hat{q}) | r'\sigma' \rangle \psi_k(r'\sigma') \quad (\text{C2})$$

into Eq. (48) and remembering the fact that, in the variation of $\psi_k(r\sigma)$, only the variation of $\phi_k(r, \sigma)$ automatically includes¹ the variation of \hat{q} one obtains up to second-order in p ,

$$\begin{aligned} \delta E = \sum_{\sigma_1 \sigma_2 k q} \int d^3r_1 d^3r_2 \delta \phi_k^*(r_1, \sigma_1) & \left\{ h \mathfrak{g}(r) \delta(r_1 - r_2) + ip \langle r_1 \sigma_1 | [h_0, \hat{q}] + \bar{h}_1 | r_2 \sigma_2 \rangle \right. \\ & \left. + \frac{i^2 p^2}{2!} \langle r_1 \sigma_1 | [[h_0, q], q] + 2[\bar{h}_1, q] + \bar{h}_2 | r_2 \sigma_2 \rangle \right\} \phi_k(r_2, \sigma_2) + \text{H.c.}, \quad (\text{C3}) \end{aligned}$$

where

$$h \mathfrak{g}(r) = -\nabla \cdot \frac{\hbar^2}{2m_q^{(0)*}(r)} \nabla + U_q^{(0)}(r) + \frac{1}{2i} [\vec{\nabla} \sigma \cdot \vec{B}_q^{(0)}(r) + \vec{B}_q^{(0)}(r) \cdot \vec{\nabla} \sigma], \quad (\text{C4a})$$

$$\bar{h} \mathfrak{q}(r) = \frac{1}{2i} [\nabla \cdot I_q^{(1)}(r) + I_q^{(1)}(r) \cdot \nabla] - \nabla \cdot (\sigma \cdot C_q^{(1)}) \nabla + \sum_q^{(1)} \cdot \sigma, \quad (\text{C4b})$$

$$\bar{h} \mathfrak{z}(r) = -\nabla \cdot \frac{\hbar^2}{2m_q^{(2)*}(r)} \nabla + U_q^{(2)} + \frac{1}{2i} [\vec{\nabla} \sigma \cdot \vec{B}_q^{(2)}(r) + \vec{B}_q^{(2)}(r) \cdot \vec{\nabla} \sigma], \quad (\text{C4c})$$

where the zeroth-, first-, and second-order quantities $m^{(0,2)*}$, $U^{(0,2)}$, $\vec{B}^{(0,2)}$, $I^{(1)}$, $C^{(1)}$, $\sum^{(1)}$ are obtained by expanding m^* , U , B , I , C , and \sum in powers of p with the use of Eqs. (42).

-
- ¹F. Villars, Nucl. Phys. **A285**, 269 (1977).
²M. Baranger and M. Vénéroni, Ann. Phys. **114**, 123 (1978).
³K. Goeke and P. G. Reinhard, Ann. Phys. **112**, 328 (1978).
⁴A. K. Mukherjee and M. K. Pal, Nucl. Phys. **A373**, 289 (1982).
⁵A. K. Mukherjee and M. K. Pal, Phys. Lett. **100B**, 457 (1981).
⁶A. K. Mukherjee and M. K. Pal, Pramana **24**, 109 (1985).
⁷A. K. Mukherjee, Phys. Rev. C **42**, 1141 (1990).
⁸S. Krewald, V. Klemt, J. Speth, and A. Faessler, Nucl. Phys. **A281**, 166 (1977).
⁹K. Goeke, P. G. Reinhard, and J. A. Maruhn, Phys. Rev. Lett. **44**, 1740 (1980).
¹⁰K. Goeke, F. Grümmer, and P. G. Reinhard, Phys. Lett. **124**, 21 (1983).
¹¹K. Goeke, F. Grümmer, and P. G. Reinhard, Ann. Phys. **150**, 504 (1983).
¹²B. Slavov, F. Grümmer, K. Goeke, R. Gissler, V. I. Dimitrov, and Ts. Venkova, J. Phys. G **16**, 395 (1990).
¹³H. Flocard, P. H. Heenen, and D. Vautherin, Nucl. Phys. **A339**, 336 (1980).
¹⁴J. W. Negele, Rev. Mod. Phys. **54**, 913 (1982), and references therein.
¹⁵J. Okolowicz, J. M. Irvine, and J. Nemeth, J. Phys. G **9**, 1385 (1983); **G 11**, 721 (1985).
¹⁶J. Okolowicz and J. M. Irvine, J. Phys. G **13**, 1399 (1987).
¹⁷P. Bonche, H. Flocard, P. H. Heenen, S. J. Krieger, and M. S. Weiss, Nucl. Phys. **A443**, 39 (1985).
¹⁸N. Redon, J. Meyer, M. Meyer, P. Quentin, M. S. Weiss, P. Bonche, H. Flocard, and P. H. Heenen, Phys. Lett. B **181**, 185 (1986).
¹⁹P. Bonche, S. J. Krieger, P. Quentin, M. S. Weiss, J. Meyer, M. Meyer, N. Redon, H. Flocard, and P. H. Heenen, Nucl. Phys. **A500**, 308 (1989).
²⁰J. F. Berger, M. Girod, and D. Gogny, Nucl. Phys. **A428**, 23c (1984); **A502**, 85c (1989).
²¹T. H. R. Skyrme, Nucl. Phys. **9**, 615 (1959).
²²P. Quentin and H. Flocard, Annu. Rev. Nucl. Sci. **28**, 523 (1978).
²³D. M. Brink and D. Vautherin, Phys. Rev. C **5**, 626 (1972).
²⁴Y. M. Engel, D. M. Brink, K. Goeke, S. J. Krieger, and D. Vautherin, Nucl. Phys. **A249**, 215 (1975).
²⁵A. K. Mukherjee and M. K. Pal, in *TDHF and Beyond*, Vol. 171 of *Lecture Notes in Physics*, edited by K. Goeke and P. G. Reinhard (Springer-Verlag, Berlin, 1982), p. 358.
²⁶M. K. Pal, *Theory of Nuclear Structure* (Affiliated East-West, New Delhi, 1982).
²⁷P. R. Halmos, *Finite Dimensional Vector Spaces* (Princeton University, Princeton, 1955).
²⁸A. K. Mukherjee, Ph.D. thesis, Calcutta University, 1989.
²⁹A. K. Kerman and S. E. Koonin, Ann. Phys. **100**, 332 (1976).
³⁰A. K. Mukherjee, Phys. Rev. C **43**, 912 (1991).