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TIME-DEPENDENT HARTREE-FOCK THEORY
WITH SKYRME'S INTERACTION

Y. M. ENGEL, D. M. BRINK and K. GOEKE[†]

Department of Theoretical Physics, University of Oxford, Oxford, England

S. J. KRIEGER[††]

Nuclear Physics Laboratory, Oxford, England

and

D. VAUTHERIN

Institut de Physique Nucléaire, Division de Physique Théorique,
91406 − Orsay, France[†††]

Abstract: The time-dependent Hartree-Fock theory (TDHF) and its adiabatic approximation (ATDHF) are formulated in coordinate space using effective density-dependent interactions of Skyrme type. For this purpose it is necessary to derive the energy density of a Slater determinant without assuming the single-particle states to be invariant under time-reversal. The corresponding Hartree-Fock Hamiltonian is obtained by varying the total energy with respect to the single-particle density matrix. With the Skyrme interaction TDHF theory leads to an equation of continuity for the single-particle density. The ATDHF equation is transformed into a finite set of inhomogeneous differential equations. Hydrodynamic-like expressions for the collective kinetic energy are established in case the single-particle wave functions have certain generalised scaling properties. TDHF and ATDHF are applied to the description of isoscalar monopole vibrations in ^{16}O and ^{40}Ca.

1. Introduction

In recent years there has been renewed interest in microscopic theories of collective motion which are able to handle processes with large amplitude. Such theories are needed in studying the dynamics of processes like fission, heavy-ion reactions and collective vibrations of soft nuclei. In each of these cases, the random-phase approximation (RPA) is obviously of no help, since it can only deal with small harmonic vibrations around the Hartree-Fock minimum. For this reason it is necessary to return to the earlier and more general formulations of nuclear collective motion. Among these, we would like to mention the resonating group method [1]), the generator coordinate method [2]), and the time-dependent Hartree-Fock method (TDHF), which was introduced by Dirac in 1931 [ref. [3])].

In this present paper we consider one of the previous theories, namely the time-dependent Hartree-Fock theory, and also its adiabatic limit which was worked out by

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[†] On leave from the Institut für Kernphysik, Kernforschungsanlage Jülich, D-517 Jülich, West Germany.

[††] On leave from the University of Illinois at Chicago Circle, Illinois 60680, USA.

[†††] Laboratoire Associé au Centre National de la Recherche Scientifique.

Belyaev [4]), Villars [5]), and Baranger and Vénéroni [6]). Our aim is to investigate this method in the case of Skyrme's interaction [7]). Let us recall that this force has proved to be very useful in Hartree-Fock calculations [8-10]) because of its computational simplicity and also because it provides a very good description of many nuclear ground state properties in spherical nuclei as well as in deformed nuclei. TDHF is also an average field approximation and the Skyrme interaction might also be appropriate in this case [11]). In the present paper we show that Skyrme's interaction leads to significant simplifications also in the TDHF equations and in the adiabatic time-dependent Hartree-Fock equations (ATDHF). As a result the ATDHF equations require only a limited amount of numerical work to be amenable to practical calculations. The case of isoscalar monopole vibrations is discussed as an illustration.

In sect. 2 we present for completeness a brief review of time-dependent Hartree-Fock theory and discuss its relationship to the random phase approximation and to the ATDHF approximation. Sect. 3 concerns the time-reversal properties of the density matrix which are necessary to derive the TDHF equation for Skyrme's interaction. This derivation is carried out in sect. 4, while in sect. 5 we demonstrate that the equation of motion leads to a continuity equation for the single-particle density and for the current density. In sects. 6 and 7 the adiabatic time-dependent Hartree-Fock equation is derived for Skyrme's interaction and is shown to reduce to a rather simple form in coordinate space. The TDHF and ATDHF methods are applied to the calculation of isoscalar monopole vibrations in sects. 8 and 9 respectively. In particular, we prove in sect. 9 that if the collective variable is a scaling variable, the mass parameter can be calculated analytically and is identical to the hydrodynamical result. Numerical results are presented and discussed in sect. 10 and sect. 11 gives a short summary of our main conclusions.

2. Time-dependent Hartree-Fock theory

Time-dependent Hartree-Fock theory (TDHF) describes the nucleus by a Slater determinant or equivalently by a density matrix $\rho(r, r')$ both being time-dependent. The density matrix ρ has the HF property $\rho^2 = \rho$. Using the Heisenberg equation one obtains with Wick's theorem the equation of motion

$$i\hbar \frac{\partial \rho}{\partial t} = [W, \rho] \qquad \text{(TDHF)}, \qquad (2.1)$$

where

$$W = K + \text{Tr} V \rho \qquad (2.2)$$

is the HF Hamiltonian. It is obtained by varying the expectation value E of the total Hamiltonian with respect to ρ,

$$\delta E = \text{Tr}(W \delta \rho). \qquad (2.3)$$

In eq. (2.2) K represents the one-body terms and V the effective two-body interaction.

The TDHF equation (2.3) is a generalisation of the static HF equation

$$[W, \rho_{HF}] = 0 \quad \text{(HF)}. \tag{2.4}$$

For doubly even nuclei the static HF density ρ_{HF} is normally even under time-reversal. However, in TDHF ρ must contain both time-even and time-odd components in order to satisfy eq. (2.1).

The random phase approximation (RPA) can be derived from the TDHF equation by limiting the collective motion to small oscillations around the static HF minimum

$$\rho \approx \rho_{HF} + \bar{\rho}, \tag{2.5}$$

with $\bar{\rho}$ being of first order small compared to the time-independent ρ_{HF}. The resulting equation for $\bar{\rho}$,

$$i\hbar \frac{\partial \bar{\rho}}{\partial t} = [\bar{W}, \rho_{HF}] + [W_{HF}, \bar{\rho}] \quad \text{(RPA)}, \tag{2.6}$$

is one representation of the RPA equations [12]), with W_{HF} and $\bar{W}$ defined analogously to eq. (2.2). Both the time-even and time-odd parts of $\bar{\rho}$ are assumed to be small. According to ref. [6]) these are connected to the collective amplitudes and the collective velocities respectively.

One step beyond the RPA approach consists in assuming that the collective velocities are small compared to single-particle velocities with no restriction on the amplitude. This is the adiabatic time-dependent Hartree-Fock approach (ATDHF). In terms of the density matrix

$$\rho \approx \rho_0 + \rho_1, \tag{2.7}$$

where ρ_1 is the time-odd part of the density matrix. It is assumed to be small compared to the time-even part ρ_0. The resulting ATDHF equation for ρ_1 is (see sect. 6)

$$i\hbar \frac{\partial \rho_0}{\partial t} = [W_0, \rho_1] + [W_1, \rho_0] \quad \text{(ATDHF)}, \tag{2.8}$$

with W_0 and W_1 defined in analogy to eq. (2.2), with ρ replaced by ρ_0 and ρ_1 respectively.

One can see how this way of introducing adiabacity is connected with assuming the collective velocity v_{coll} smaller than Fermi velocity v_F, i.e. $v_{coll} \ll v_F$. For nuclear systems $\hbar k_F r_0 \approx 1$ with $r_0 = 1.2$ fm and k_F is the Fermi momentum. If we write A for the amplitude and ω for the angular frequency of the collective motion, then $v_{coll} \approx A\omega$ and the inequality becomes

$$\hbar\omega A \ll \hbar v_F \approx 2r_0 \varepsilon_F, \tag{2.9}$$

with ε_F denoting the Fermi energy. If $\hbar\omega \ll \varepsilon_F$ the adiabatic condition $v_{coll} \ll v_F$ can be satisfied even with a large amplitude motion, $A > r_0$, but if the collective frequency is large $\hbar\omega \approx \varepsilon_F$ then the adiabatic condition requires that the amplitude should be small, $A \ll r_0$. In this case ATDHF is equivalent to RPA.

There are various previous attempts to solve the TDHF equations by means of adiabatic approaches, which are not equivalent to ATDHF. Authors like Bar-Touv [ref. [13])] and Wong [ref. [14])] use the cranking technique. Baranger and Kumar [15]) start with the full ATDHF theory. Because they use a separable interaction neglecting exchange effects, the term $[W_1, \rho_0]$ does not appear in their equations and their result for the effective mass reduces to the cranking model.

3. Properties of the single-particle density matrix under time-reversal

The explicit expression of W for Skyrme's interaction was derived in ref. [9]) in the case of the static Hartree-Fock problem, i.e. assuming time-reversal invariance. However, in a time-dependent problem it is clear from eq. (2.1) that ρ cannot be time-even. As a consequence, the form of W must be generalised to include contributions from time-odd parts of ρ. This generalization will be performed in sect. 4. In the present section we investigate first the time-reversal properties of the density matrix ρ.

We denote the single-particle orbitals by $\Phi_k(r\sigma q)$ where $\sigma = \pm\frac{1}{2}$ and $q = \pm\frac{1}{2}$ are the spin and isospin coordinates. We consider only cases where the single-particle density is diagonal in q, and therefore

$$\rho_q(r\sigma, r'\sigma') = \sum_k \Phi_k(r\sigma q)\Phi_k^*(r'\sigma'q) = \langle r\sigma q|\hat{\rho}|r'\sigma'q\rangle, \tag{3.1}$$

where the sum is restricted to occupied orbitals. This definition agrees with that of Villars [16]) and Thouless [17]), and is the Hermitian conjugate to that of Negele and Vautherin [18]). For notational convenience we shall omit the isospin coordinate q in this section. We write the time-reversal operator

$$K = -i\sigma_y K_0,$$

where K_0 denotes the complex conjugation and σ_y is a Pauli spin matrix. Thus the time-reverse of a state Φ_i is

$$K\Phi_i(r\sigma) = -2\sigma\Phi_i^*(r-\sigma),$$

and the time-reversed density matrix

$$\rho^T(r\sigma, r'\sigma') = \sum_i K\Phi_i(r\sigma)K\Phi_i^*(r'\sigma') \tag{3.2}$$

$$= 4\sigma\sigma'\rho(r'-\sigma', r-\sigma).$$

As ρ is also Hermitian, i.e.

$$\rho^*(r\sigma, r'\sigma') = \rho(r'\sigma', r\sigma),$$

eq. (3.2) can also be written as

$$\rho^T(r\sigma, r'\sigma') = 4\sigma\sigma'\rho^*(r-\sigma, r'-\sigma'). \tag{3.3}$$

The complete density matrix can be written in terms of a scalar part $\rho(r, r')$ and a vector part $s(r, r')$, both being hermitian,

$$\rho(r\sigma, r'\sigma') = \tfrac{1}{2}[\rho(r, r')\delta_{\sigma\sigma'} + \sum_v (\sigma|\sigma_v|\sigma')s_v(r, r')], \tag{3.4}$$

where

$$\rho(r, r') = \sum_\sigma \rho(r\sigma, r'\sigma),$$

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

According to eq. (3.3) the scalar and vector parts $\rho^T(r, r')$ and $s^T(r, r')$ of the time-reversed density matrix $\rho^T(r\sigma, r'\sigma')$ are

$$\rho^T(r, r') = \rho^*(r, r') = \rho(r', r), \tag{3.5}$$

$$s^T(r, r') = -s^*(r, r') = -s(r', r). \tag{3.6}$$

In sect. 4 we need various special densities which can be constructed from the single-particle density matrix. They are:

(i) particle density,

$$\rho(r) = \rho(r, r), \tag{3.7}$$

(ii) kinetic energy density,

$$\tau(r) = [\nabla \cdot \nabla'\rho(r, r')]_{r=r'}, \tag{3.8}$$

(iii) spin density,

$$s(r) = s(r, r), \tag{3.9}$$

(iv) momentum density,

$$j(r) = \frac{1}{2i}[(\nabla - \nabla')\rho(r, r')]_{r=r'}, \tag{3.10}$$

(v) spin current tensor,

$$J_{\mu v}(r) = \frac{1}{2i}[(\nabla_\mu - \nabla'_\mu)s_v(r, r')]_{r=r'}, \tag{3.11}$$

(vi) kinetic energy density (vector part)

$$T(r) = [\nabla \cdot \nabla's(r, r')]_{r=r'}. \tag{3.12}$$

These densities are all real. Denoting by an index T the densities corresponding to $\rho^T(r\sigma, r'\sigma')$ one finds the following transformation properties under time-reversal

$$\rho^T(r) = \rho(r), \quad \tau^T(r) = \tau(r), \quad J_{\mu v}^T(r) = J_{\mu v}(r),$$
$$s^T(r) = -s(r), \quad j^T(r) = -j(r), \quad T^T(r) = -T(r). \tag{3.13}$$

In a static situation the density matrix $\rho(r\sigma, r'\sigma')$ is invariant under time-reversal, which implies $j^T = j$, $s^T = s$ and $T^T = T$. Thus the transformation properties (3.13) require that j, s and T are zero. The spin-orbit density $J(r)$ introduced in ref. [9]) is the

antisymmetric part of the tensor $J_{\mu\nu}(r)$:

$$J(r) = \frac{1}{2i}[(\nabla - \nabla') \times s(r, r')]_{r=r'}.$$

4. Energy density and Hartree-Fock Hamiltonian with Skyrme's interaction

Skyrme's interaction [7]) consists of a two-body term $v^{(2)}$ including a spin-orbit potential, and a three-body term, $v^{(3)}$:

$$V = \sum_{i<j} v^{(2)}_{ij} + \sum_{i<j<k} v^{(3)}_{ijk}.$$

In the coordinate space representation, $v^{(2)}$ and $v^{(3)}$ are

$$v^{(2)}(r_1, r_2) = t_0(1 + x_0 P_\sigma)\delta(r_1 - r_2) + \tfrac{1}{2}t_1[\delta(r_1 - r_2)k^2 + k'^2\delta(r_1 - r_2)]$$

$$+ t_2 k' \cdot \delta(r_1 - r_2)k + iV_{\text{s.o.}}(\sigma_1 + \sigma_2) \cdot k' \times \delta(r_1 - r_2)k, \tag{4.1}$$

$$v^{(3)}(r_1, r_2, r_3) = t_3\delta(r_1 - r_2)\delta(r_2 - r_3). \tag{4.2}$$

In eq. (4.1) P_σ is the spin exchange operator and σ represents the vector of the Pauli spin matrices; k is the operator $(1/2i)(\nabla_1 - \nabla_2)$ acting on the right and k' is $-(1/2i)$ $(\nabla_1 - \nabla_2)$ acting on the left. Here x_0, t_0, t_1, t_2, t_3 and the spin-orbit coupling strength $V_{\text{s.o.}}$ are parameters of the interaction. As in ref. [9]) the expectation value E of the many-particle Hamiltonian can be written as an integral of an energy density $H(r)$

$$E = \int d^3r\, H(r). \tag{4.3}$$

The full expression for $H(r)$ is derived in appendix A. It depends on all the densities (3.7)–(3.12) and reduces to the corresponding expression in ref. [9]) when the density matrix is time-even.

For clarity we discuss in this paragraph the special case of a spin saturated and charge conjugated nucleus (i.e. $\rho_p = \rho_n = \tfrac{1}{2}\rho$, etc.). In this case eq. (A.19) reduces to

$$H(r) = \frac{\hbar^2}{2m}\tau + \tfrac{3}{8}t_0\rho^2 + \tfrac{1}{16}(3t_1 + 5t_2)(\rho\tau - j^2) - \tfrac{1}{64}(9t_1 - 5t_2)\rho\nabla^2\rho + \tfrac{1}{16}t_3\rho^3. \tag{4.4}$$

The new feature in eq. (4.4) is the appearance of the momentum density $j(r)$. It occurs in the combination $\rho\tau - j^2$. This is sufficient for the potential energy expectation value to be Galilean invariant and reflects the Galilean invariance of the Skyrme interaction. A Galilean transformation replaces a single-particle wave function, $\Phi(r, \sigma)$ by $e^{ik\cdot r}\Phi(r, \sigma)$. Thus the density matrix transforms to

$$\tilde{\rho}(r, r') = e^{ik\cdot(r-r')}\rho(r, r'), \tag{4.5}$$

$$\tilde{\tau}(r) = \tau(r) + 2k \cdot j(r) + k^2, \tag{4.6}$$

$$\tilde{j}(r) = j(r) + k\rho(r). \tag{4.7}$$

The transformation (4.5)–(4.7) leaves $\rho\tau - j^2$ invariant.

The variation of the energy density yields the expression for the Hamiltonian W. The general expressions are derived in appendix B. In case of a spin saturated nucleus (but not necessarily $N = Z$) and neglecting spin-orbit and Coulomb effects, eqs. (B.16)–(B.18) reduce to

$$W_q(\mathbf{r}) = -\mathbf{\nabla} \cdot \frac{\hbar^2}{2m_q^*(\mathbf{r})}\,\mathbf{\nabla} + U_q(\mathbf{r}) + \frac{1}{2i}(\mathbf{\nabla} \cdot \mathbf{I}_q + \mathbf{I}_q \cdot \mathbf{\nabla}), \tag{4.8}$$

with

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = \frac{\hbar^2}{2m} + \tfrac{1}{4}(t_1 + t_2)\rho + \tfrac{1}{8}(t_2 - t_1)\rho_q, \tag{4.9}$$

$$U_q(\mathbf{r}) = t_0[(1 + \tfrac{1}{2}x_0)\rho - (x_0 + \tfrac{1}{2})\rho_q] + \tfrac{1}{8}(t_2 - 3t_1)\mathbf{\nabla}^2\rho + \tfrac{1}{16}(3t_1 + t_2)\mathbf{\nabla}^2\rho_q + \tfrac{1}{4}(t_1 + t_2)\tau$$
$$+ \tfrac{1}{8}(t_2 - t_1)\tau_q + \tfrac{1}{4}t_3(\rho^2 - \rho_q^2), \tag{4.10}$$

$$\mathbf{I}_q(\mathbf{r}) = -\tfrac{1}{2}(t_1 + t_2)\mathbf{j} - \tfrac{1}{4}(t_2 - t_1)\mathbf{j}_q. \tag{4.11}$$

Again the term containing the momentum densities $\mathbf{j}$ and $\mathbf{j}_q$ is new and does not appear in the static HF case. Notice that due to Galilean invariance they appear with the same coefficients as the terms determining the density dependence of the effective mass.

5. Equation of continuity

The TDHF equation leads in the case of velocity and density independent interactions to a continuity equation for the total particle density ρ [see for example ref. [19]]. We will now show that this equation still holds in the case of the Skyrme interaction. For this purpose let us consider first the spin independent part of the Hamiltonian [see eq. (4.8)]. In calculating, in coordinate space, the diagonal part of $i\hbar\dot{\rho}_q = [W_q, \rho_q]$ the following terms will occur:

(i) $[U, \rho]_{r = r'} = [(U(\mathbf{r}) - U(\mathbf{r}'))\rho(\mathbf{r}, \mathbf{r}')]_{r = r'} = 0;$

(ii) $\left[\mathbf{\nabla} \cdot \dfrac{1}{m^*(\mathbf{r})}\mathbf{\nabla}, \rho\right]_{r = r'} = \left[\left(\mathbf{\nabla} \cdot \dfrac{1}{m^*(\mathbf{r})}\mathbf{\nabla} - \mathbf{\nabla}' \cdot \dfrac{1}{m^*(\mathbf{r}')}\mathbf{\nabla}'\right)\rho(\mathbf{r}, \mathbf{r}')\right]_{r = r'}$

$\qquad = \left(\mathbf{\nabla}\dfrac{1}{m^*(\mathbf{r})}\right) \cdot (\mathbf{\nabla} - \mathbf{\nabla}')\rho(\mathbf{r}, \mathbf{r}')\Big|_{r = r'} + \dfrac{1}{m^*(\mathbf{r})}(\mathbf{\nabla} + \mathbf{\nabla}') \cdot (\mathbf{\nabla} - \mathbf{\nabla}')\rho(\mathbf{r}, \mathbf{r}')\Big|_{r = r'}$

$\qquad = 2i\mathbf{\nabla} \cdot \left(\dfrac{1}{m^*(\mathbf{r})}\mathbf{j}(\mathbf{r})\right);$

(iii) $[\mathbf{\nabla} \cdot \mathbf{j} + \mathbf{j} \cdot \mathbf{\nabla}, \rho]_{r = r'} = [(\mathbf{\nabla} \cdot \mathbf{j}) + 2\mathbf{j} \cdot \mathbf{\nabla}, \rho]_{r = r'} = [2\mathbf{j} \cdot \mathbf{\nabla}, \rho]_{r = r'}$

$\qquad = 2(\mathbf{j}(\mathbf{r}) \cdot \mathbf{\nabla}\rho(\mathbf{r}, \mathbf{r}') - \rho(\mathbf{r}, \mathbf{r}')\mathbf{j}(\mathbf{r}') \cdot \mathbf{\nabla}')_{r = r'}.$

Integration by parts on the second term yields

$$2(j(r) \cdot \nabla\rho(r, r')+j(r) \cdot \nabla'\rho(r, r')+\rho(r, r')\nabla' \cdot j(r'))_{r=r'}$$

$$= 2(j(r) \cdot \nabla\rho(r)+\rho(r)\nabla \cdot j(r)) = 2\nabla \cdot (\rho j).$$

Collecting the terms and substituting into the diagonal part of the TDHF equation gives

$$\frac{\partial\rho_q}{\partial t} + \frac{\hbar}{m} \nabla \cdot j_q = \frac{1}{2\hbar} (t_1+t_2)\nabla \cdot (\rho_q j-\rho j_q). \tag{5.1}$$

The term on the right hand side of eq. (5.1) comes from the exchange forces and expresses the fact that proton and neutron densities can change by exchange of protons and neutrons as well as by physical movement of the particles.

If spin terms are included, there will be an extra term on the right hand side of eq. (5.1), which is derived in a similar way

$$\frac{V_{\text{s.o.}}}{2\hbar} \nabla \cdot (\rho_q\nabla \times s-\rho\nabla \times s_q). \tag{5.2}$$

For the case of a $T = 0$ mode in a self-conjugate nucleus $(\rho_q = \frac{1}{2}\rho, j_q = \frac{1}{2}j)$ the right hand sides of (5.1) and (5.2) are zero and we have the usual form of the continuity equation.

An equation of continuity for the total particle density $\rho = \rho_p+\rho_n, j = j_p+j_n$ and $s = s_p+s_n$ is obtained by adding equation (5.1) for protons and neutrons. The contributions from the right hand side cancel, giving

$$\frac{\partial\rho}{\partial t} + \frac{\hbar}{m} \nabla \cdot j = 0. \tag{5.3}$$

For an adiabatic motion the analogous equation of continuity can easily be derived in the same way if one starts from eq. (2.8) instead of eq. (2.1):

$$\frac{\partial\rho_0}{\partial t} + \frac{\hbar}{m} \nabla \cdot j_1 = 0, \tag{5.4}$$

where j_1 is $(1/2i) (\nabla - \nabla') \rho_1 (r, r')|_{r=r'}$, $\rho_1 (r, r')$ being defined in the next section.

6. The adiabatic approximation

Following Baranger and Vénéroni [6]), we split the HF density ρ, and the HF Hamiltonian W, into their time-even and time-odd components:

$$\rho = \rho_+ +\rho_- , \tag{6.1}$$

$$W = W_+ +W_- . \tag{6.2}$$

The time-odd part of eq. (2.1) then reads

$$i\hbar\dot{\rho}_+ = [W_+, \rho_-] + [W_-, \rho_+]. \tag{6.3}$$

In order to made the division between the time-even and time-odd components it is convenient to write [6])

$$\rho = e^{i\chi}\rho_0 e^{-i\chi}, \tag{6.4}$$

where both ρ_0 and χ are Hermitian and time-even and ρ_0 is a Slater determinant, i.e. $\rho_0^2 = \rho_0$. In order to define ρ_0 and χ in a unique way the further conditions $\rho_0\chi\rho_0 = (1-\rho_0)\chi(1-\rho_0) = 0$ are also required [6]). These conditions imply that χ has only particle-hole matrix elements with respect to ρ_0. The adiabatic approximation then consists in expanding eq. (6.4) as a power series in the "velocity" χ,

$$\rho = \rho_0 + i[\chi, \rho_0] + \tfrac{1}{2}i^2[\chi, [\chi, \rho_0]] + \dots, \tag{6.5}$$

and stopping at second order. We define

$$\rho_1 = i[\chi, \rho_0], \tag{6.6}$$

$$\rho_2 = \tfrac{1}{2}i^2[\chi, [\chi, \rho_0]]. \tag{6.7}$$

The lowest order approximation to eq. (6.3) is

$$i\hbar\dot{\rho}_0 = [W_0, \rho_1] + [W_1, \rho_0]. \tag{6.8}$$

Eq. (6.8) is an equation for the time-odd density ρ_1 in terms of $\dot{\rho}_0$.

Since χ has only particle-hole matrix elements, then $\chi = i[\rho_0, \rho_1]$ and ρ_2 may be written in terms of ρ_1 as

$$\rho_2 = (1-\rho_0)\rho_1^2(1-\rho_0) - \rho_0\rho_1^2\rho_0. \tag{6.9}$$

Following the solution of eq. (6.8) the energy may be calculated through second order in the velocities as

$$E = \text{Tr}(W\rho)$$
$$\approx \text{Tr}(W_0\rho_0 + W_1\rho_0 + W_0\rho_1 + W_0\rho_2 + W_2\rho_0 + W_1\rho_1). \tag{6.10}$$

Due to the time-reversal invariance of the many-body Hamiltonian the terms linear in ρ_1 will not contribute and the energy thus is the sum of a potential energy,

$$\mathscr{V} = \text{Tr}(K\rho_0) + \tfrac{1}{2}\text{Tr Tr}(\rho_0 V\rho_0), \tag{6.11}$$

and a kinetic energy quadratic in χ,

$$\mathscr{K} = \text{Tr}(W_0\rho_2) + \tfrac{1}{2}\text{Tr}_1\text{Tr}_2(\rho_1(1)V(1,2)\rho_1(2)). \tag{6.12}$$

For practical applications Baranger [6]) chooses ρ_0 dependent on a few collective coordinates $\rho_0(u_1, u_2, \dots)$. In this work we suppose there is just one such parameter u. Then $\dot{\rho}_0 = \dot{u}\,\partial\rho_0/\partial u$ is linear in $\dot{u}$ and the solution χ of eq. (6.8) is also proportional

to $\dot{u}$. The potential energy $\mathcal{V}$ depends also on u whereas $\mathcal{K}$ depends on u and $\dot{u}$ and is quadratic in $\dot{u}$:

$$\mathcal{K} = \tfrac{1}{2} M(u) \dot{u}^2. \tag{6.13}$$

Eq. (6.13) defines the collective mass $M(u)$.

The kinetic energy $\mathcal{K}$ can be written in a simpler form if one uses (6.8), (6.9) and $\rho_1 = \rho_0 \rho_1 + \rho_1 \rho_0$ and $\chi = i[\rho_0, \rho_1]$:

$$\mathcal{K} = \tfrac{1}{2} \hbar \, \mathrm{Tr} \, (\chi \dot{\rho}_0). \tag{6.14}$$

In fact we may write $\dot{\rho}_0$ as $\dot{u} \, \partial \rho_0 / \partial u$. Then comparison of eq. (6.14) with the classical expression $\mathcal{K} = \tfrac{1}{2} p \dot{u}$ suggests that

$$p = \hbar \, \mathrm{Tr} \left(\chi \frac{\partial \rho_0}{\partial u} \right) \tag{6.15}$$

can be considered as the momentum conjugate to u. Since χ is a linear function of $\dot{u}$ we have

$$p = M(u) \dot{u}, \tag{6.16}$$

which gives again the mass parameter. The classical Hamiltonian can therefore be written

$$H(p, u) = \frac{1}{2M(u)} p^2 + \mathcal{V}(u). \tag{6.17}$$

This Hamiltonian can be quantized to give the collective energy levels.

7. ATDHF with Skyrme's interaction

In order to obtain the effective mass one has to solve the ATDHF equation (6.8) which gives ρ_1 in terms of $\dot{\rho}_0$. We will show now that the formulation of W_0 and W_1 in the coordinate space using Skyrme's interaction makes eq. (6.8) no more difficult to solve than the usual HF problem with the same type of forces. The expressions for W_0 and W_1 are derived in appendix B. If we write

$$\rho_0(r, r') = \sum_M \phi_M(r) \phi_M^*(r'), \tag{7.1}$$

then from $\rho_1 = \rho_0 \rho_1 + \rho_1 \rho_0$, it is easy to show that ρ_1 can be written as

$$\rho_1(r, r') = i \sum_M [\eta_M(r) \phi_M^*(r') - \phi_M(r) \eta_M^*(r')], \tag{7.2}$$

where $\eta_M(r) = \int d^3 r' \rho_1(r, r') \phi_M(r')$ is orthogonal to all occupied states $\phi_N(r)$. It is also a condition of the theory [6]) that $[W_0, \rho_0]$ is small, of second order in χ; therefore, approximately, the ϕ_M are eigenstates of W_0 with eigenvalue ε_M. Hence one obtains the following expression for $\eta_M(r)$ if one multiplies the ATDHF equation (6.8)

from right by $\phi_N(r')$ and integrates over d^3r':

$$(W_0 - \varepsilon_N)\eta_N(r) = i \int \dot{\rho}_0(r, r')\phi_N(r')d^3r' - \int \langle r|[W_1, \rho_0]|r'\rangle\phi_N(r')d^3r'. \quad (7.3)$$

With the Skyrme interaction eq. (7.3) is an inhomogeneous differential equation for the unknown function $\eta_N(r)$ with the boundary condition that $\eta_N(r)$ is regular and goes to zero for $r \to \infty$ and $\langle \eta_N|\phi_M\rangle = 0$ for all occupied states ϕ_M. However, the inhomogeneity on the right hand side of eq. (7.3) contains the unknown $\eta_N(r)$ via the momentum currents appearing in W_1. Therefore, an iterative procedure is appropriate, which may start with the cranking term, i.e. assuming $W_1 = 0$. In addition for isoscalar modes in spherical self-conjuncted nuclei the W_1 depends just on j (see appendix B), where j is known from the equation of continuity. In such a case eq. (7.3) can be solved directly without iteration. Altogether, eq. (7.3) is not expected to be more difficult to solve than the corresponding Hartree-Fock single-particle equation. It should be emphasised at this point that the coordinate representation allows the ATDHF equation to be solved without expanding $\eta_N(r)$ into wave functions of particle states of the Hartree-Fock solution, which are usually unbound. This method, therefore, avoids the problems of discretizing continuum states [20]).

8. TDHF applied to monopole vibrations

As an application of the TDHF method discussed above we consider in the present section a simple time-dependent variational calculation of the isoscalar monopole mode in ^{16}O with the Skyrme interaction. At each time we assume the system to be described by a Slater determinant $|\psi\rangle$. Then the TDHF equations can be derived [21]) from the variational principle

$$\delta I = 0, \quad \text{where} \quad I = \int_{t_0}^{t_1} dt \langle \psi|i\hbar \frac{\partial}{\partial t} - H|\psi\rangle. \quad (8.1)$$

In the present section we solve the variational eq. (8.1) by assuming that ψ is a Slater determinant of pure harmonic oscillator functions. In order to describe non-stationary states we introduce time-odd components in the wave functions $|\psi(b)\rangle$ by allowing the oscillator parameter b to be complex [22]):

$$\frac{1}{b(t)} = \alpha(t) + i\beta(t). \quad (8.2)$$

Using as independent variables $\delta = \alpha\beta$ and $\gamma = \sqrt{\alpha^2 - \beta^2}$ we have in the case of ^{16}O the two normalized radial wave functions

$$u_{0s}(r) = \left(\frac{4\gamma^3}{\sqrt{\pi}}\right)^{\frac{1}{4}} e^{-\frac{1}{2}r^2\gamma^2} e^{-i\delta r^2} \equiv \bar{u}_{0s}(r)e^{-i\delta r^2},$$

$$u_{0p}(r) = \left(\frac{8\gamma^5}{3\sqrt{\pi}}\right)^{\frac{1}{4}} re^{-\frac{1}{2}r^2\gamma^2} e^{-i\delta r^2} \equiv \bar{u}_{0p}e^{-i\delta r^2}. \quad (8.3)$$

It may be noticed that the radial wave functions are equal to $e^{-i\delta r^2}$ times pure oscillator wave functions with the oscillator parameter γ. The quantity γ is related to the rms radius R of ^{16}O by $R = 3/2\gamma$. For the evaluation of (8.1) we used the expectation value of $i\hbar\, \partial/\partial t = i\hbar(\dot\gamma\, \partial/\partial\gamma + \dot\delta\, \partial/\partial\delta)$:

$$\langle\psi(b)|i\hbar\frac{\partial}{\partial t}|\psi(b)\rangle = i\hbar\left[4\langle u_{0s}|\frac{\partial}{\partial t}|u_{0s}\rangle + 12\langle u_{0p}|\frac{\partial}{\partial t}|u_{0p}\rangle\right] = (36/\gamma^2)\hbar\dot\delta. \tag{8.4}$$

For the calculation of $\langle\psi(b)|\hat H|\psi(b)\rangle$ we use eq. (4.4) for the energy density. The single-particle density ρ depends only on γ, and therefore $\rho = \bar\rho$. The kinetic energy density can be written as $\tau(r) = \bar\tau(r) + 4\delta^2 r^2\bar\rho(r)$. Here $\bar\tau$ and $\bar\rho$ are constructed from $\bar u_{0s}$ and $\bar u_{0p}$. One also has the property $\rho\tau - j^2 = \bar\rho\bar\tau$. Therefore the total energy is

$$E = \int H(r)\mathrm{d}^3r + 4\delta^2\frac{\hbar}{2m}\int r^2\bar\rho(r)\mathrm{d}^3r. \tag{8.5}$$

The first term is just the expectation value of the energy calculated with the real oscillator functions $\bar u_{0s}$ and $\bar u_{0p}$ [ref. [7])],

$$B(\gamma) = \frac{69}{2}\frac{\hbar^2}{2m}\gamma^2 + \frac{93}{2(2\pi)^{\frac{3}{2}}}t_0\gamma^3 + \frac{15}{4(2\pi)^{\frac{3}{2}}}(21t_1 + 16t_2)\gamma^5 + \frac{464}{9(\pi\sqrt{3})^3}t_3\gamma^6. \tag{8.6}$$

The second term of (8.5) is connected with the rms radius and is equal to $(144/\gamma^2)$ $(\hbar^2/2m)\delta^2$ so that the functional of eq. (8.1) is

$$I(\gamma(t),\delta(t)) = \int_{t_0}^{t_1}\mathrm{d}t\left\{\frac{36}{\gamma^2}\left(\hbar\dot\delta - 4\frac{\hbar^2}{2m}\delta^2\right) - B(\gamma)\right\}. \tag{8.7}$$

By varying eq. (8.7) we obtain the following equations:

$$\dot\gamma = 4\left(\frac{\hbar}{2m}\right)\gamma\delta, \tag{8.8}$$

$$\dot\delta = 4\left(\frac{\hbar}{2m}\right)\delta^2 - \frac{1}{\hbar}\frac{\gamma^3}{72}\frac{\mathrm{d}}{\mathrm{d}\gamma}B(\gamma). \tag{8.9}$$

From these equations the expectation value (8.5) of the energy,

$$\langle\psi(b)|\hat H|\psi(b)\rangle = \frac{36}{\gamma^2}\frac{\hbar^2}{2m}4\delta^2 + B(\gamma), \tag{8.10}$$

is a constant of motion. After eliminating δ from (8.10) by (8.8) this constant of motion can be written

$$E(\gamma,\dot\gamma) = \frac{18m}{\gamma^4}\dot\gamma^2 + B(\gamma). \tag{8.11}$$

Expression (8.11) can be identified with the classical energy. In terms of the rms

radius R the total energy is

$$E(R, \dot{R}) = \tfrac{1}{2}(16m)\dot{R}^2 + B(R).$$ (8.12)

Our resulting collective mass is identical to the result of Zamick [23].

By interpreting eq. (8.12) we find that the motion is periodic with a period

$$T = 2\sqrt{18m}\int_{\gamma_{min}}^{\gamma_{max}} \frac{d\gamma}{\gamma^2\sqrt{E - B(\gamma)}}.$$ (8.13)

Since $B(\gamma)$ has a sharp minimum we may approximate $B(\gamma)$ by a parabolic expansion

$$B(\gamma) = B(\gamma_0) + \tfrac{1}{2}AK\left(\frac{\gamma - \gamma_0}{\gamma_0}\right)^2,$$ (8.14)

where A is the total nucleon number and K is the compression modulus of the finite nucleus

$$K = \frac{\gamma_0^2}{A}\left(\frac{\partial^2 B}{\partial\gamma^2}\right)_{\gamma = \gamma_0} = \frac{b_0^2}{A}\left(\frac{\partial^2 B}{\partial b^2}\right)_{b = b_0}.$$ (8.15)

Inserting eq. (8.14) into (8.13) we obtain a period independent of the total energy E,

$$T = \frac{12\pi}{\gamma_0}\sqrt{\frac{m}{AK}}.$$ (8.16)

The corresponding excitation energy of the isoscalar monopole mode in ^{16}O is

$$E_{0^+} = \hbar\omega = \tfrac{1}{6}\sqrt{AK(\hbar^2\gamma_0^2/m)},$$ (8.17)

which is identical to the hydrodynamic value [24].

9. ATDHF applied to monopole vibrations

In the present section we are going to calculate the collective mass of the isoscalar monopole vibration in a charge conjugated nucleus. We will assume the density matrix ρ_0 to be constructed from harmonic oscillator states. Since we make an explicit use of the scaling property of the harmonic oscillator states, we will first derive a general expression for the collective kinetic energy which will be specialized later to the monopole mode.

The density matrices $\rho_0(r, r')$ and $\rho_1(r, r')$ are given in eqs. (7.1) and (7.2) respectively. According to eq. (3.10) the momentum current is

$$j(r) = \tfrac{1}{2}\sum_M \{\phi_M^*(\nabla\eta_M) - \eta_M^*(\nabla\phi_M) - \eta_M(\nabla\phi_M)^* + \phi_M(\nabla\eta_M)^*\}.$$ (9.1)

In eqs. (9.1)–(9.5) the sum goes over occupied states only.

Since

$$\chi(r, r') = i\langle r|[\rho_0, \rho_1]|r'\rangle = \sum_M (\phi_M(r)\eta_M^*(r') + \eta_M(r)\phi_M^*(r')),$$ (9.2)

we can write the collective kinetic energy $\mathscr{K}$, eq. (6.14), as

$$\mathscr{K} = \tfrac{1}{2}\hbar \int d^3r \sum_M \left\{ \eta_M^*(r) \frac{\partial \phi_M(r)}{\partial t} + \eta_M(r) \frac{\partial \phi_M^*(r)}{\partial t} \right\}. \tag{9.3}$$

The aim in introducing scaling properties of ϕ_M is to relate the kinetic energy (9.3) directly to the current (9.1). For this purpose we consider the expression

$$\int v(r) \cdot j(r) d^3r = \tfrac{1}{2} \sum_M \Big\{ d^3r\, v(r) \cdot [\phi_M^*(r)\nabla\eta_M(r) + \phi_M(r)\nabla\eta_M^*(r) - \eta_M(r)\nabla\phi_M^*(r)$$
$$- \eta_M^*(r)\nabla\phi_M(r)], \tag{9.4}$$

where $v(r)$ is a real differentiable vector function of r. By partial integration of the first two terms on the right hand side we obtain after some rearrangements

$$\int d^3r\, v(r) \cdot j(r) = -\sum_M \int d^3r\, \eta_M^*(r)\{\tfrac{1}{2}\phi_M(r)\nabla \cdot v(r) + v(r) \cdot \nabla\phi_M(r)\}$$
$$- \sum_M \int d^3r\, \eta_M(r)\{\tfrac{1}{2}\phi_M^*(r)\nabla \cdot v(r) + v(r) \cdot \nabla\phi_M^*(r)\}. \tag{9.5}$$

We define the wave functions $\phi_M(r)$ to have the generalised scaling property, if

$$\frac{\partial \phi_M(r)}{\partial t} = -\tfrac{1}{2}\phi_M(r)\nabla \cdot v(r) - v(r) \cdot \nabla\phi_M(r). \tag{9.6}$$

Then a comparison of eq. (9.5) with (9.3) shows just

$$\mathscr{K} = \tfrac{1}{2}\hbar \int d^3r\, v(r) \cdot j(r). \tag{9.7}$$

One can apply the above formalism to the description of the isoscalar monopole vibration of a charge-conjugated nucleus, if we assume the single-particle wave functions to be eigenfunctions of the harmonic oscillator. For, if b is the oscillator length and $u = 1/b$, the scaling properties of the harmonic oscillator wave functions are given by

$$\phi_M(u, r) = u^{\frac{3}{2}} g_M(ur), \tag{9.8}$$

with g_M a known function of the product ur. Hence

$$\frac{\partial}{\partial r} \phi_M(u, r) = u^{\frac{5}{2}} g_M'(ur),$$

$$\frac{\partial}{\partial u} \phi_M(u, r) = \tfrac{3}{2} u^{\frac{1}{2}} g_M(ur) + r u^{\frac{3}{2}} g_M'(ur),$$

and finally

$$\frac{\partial}{\partial t} \phi_M(u, r) = \frac{3\dot{u}}{2u} \phi_M(u, r) + r \frac{\dot{u}}{u} \frac{\partial \phi_M(u, r)}{\partial r}. \tag{9.9}$$

This is a special case of (9.6) with

$$v(r) = -\frac{\dot{u}}{u}\,r. \tag{9.10}$$

In this case $v(r)$ can be interpreted as radial collective velocity.

One can easily show that the scaling property (9.6) leads to a continuity equation: In fact, if we multiply eq. (9.6) with $\phi_M^*(r)$ and add the complex conjugate resulting equation, we obtain after summing over all occupied states, using (7.1):

$$\frac{\partial\rho_0}{\partial t} + \nabla\cdot(\rho_0\,v) = 0. \tag{9.11}$$

Comparing eq. (9.11) with (5.4) we get up to second order

$$\nabla\cdot(\rho_0\,v) = \frac{\hbar}{m}\,\nabla\cdot j. \tag{9.12}$$

In the case of the isoscalar monopole mode both v and j are irrotational and eq. (9.12) gives

$$j = \frac{m}{\hbar}\,\rho_0\,v. \tag{9.13}$$

Substituting (9.13) into eq. (9.7) gives

$$\mathcal{K} = \tfrac{1}{2}m\int\rho_0\,v^2\mathrm{d}^3r. \tag{9.14}$$

Using eq. (9.10) for v gives for the considered monopole vibration

$$\mathcal{K} = \frac{m}{2}\,\frac{\dot{u}^2}{u^2}\,\langle r^2\rangle. \tag{9.15}$$

Eq. (9.14) suggests also an interpretation of v as a hydrodynamic velocity. In general one cannot obtain eq. (9.14), but in cases where v is irrotational then $v(r)$ is the gradient of a scalar potential f:

$$v = \nabla f, \tag{9.16}$$

and

$$\mathcal{K} = -\tfrac{1}{2}\hbar\int f\nabla\cdot j\,\mathrm{d}^3r. \tag{9.17}$$

Comparing eq. (9.17) with (9.12) one can write

$$\mathcal{K} = -\tfrac{1}{2}m\int f\nabla\cdot(\rho_0\,v)\mathrm{d}^3r, \tag{9.18}$$

which again leads to (9.14).

For ^{16}O and ^{40}Ca the value of $\langle r^2\rangle$ in eq. (9.15) is $36/u^2$ and $120/u^2$ respectively.

Therefore in terms of the rms radius $R = (\langle r^2 \rangle / A)^{\frac{1}{2}}$ the collective kinetic energy is

$$\mathscr{K} = \begin{cases} \frac{1}{2}(16m)\dot{R}^2 & \text{for } ^{16}\text{O} & (9.19) \\ \frac{1}{2}(40m)\dot{R}^2 & \text{for } ^{40}\text{Ca}. & (9.20) \end{cases}$$

Eqs. (9.19) and (9.20) are identical to the results of Zamick's model calculation [23]).

In the case of the isoscalar giant quadrupole resonance the kinetic energy can easily be calculated in the same way using eq. (9.14) and assuming scaling properties of the form $\phi_M(u, r) = F_M(x/u, y/u, u^2 z)$ and

$$v(r) = (-2x/u, -2y/u, 4zu).$$

Results concerning this mode will be published elsewhere.

It should be remarked, that eq. (9.7) requires within the framework of the ATDHF theory nothing but the scaling properties (9.6). Eq. (9.14) requires in addition the equation of continuity and that v is irrotational. The present section thus does not make use of properties of the Skyrme interaction. A similar definition of the scaling properties has already been used in ref. [2]).

10. Results

If the collective variable is taken to be the oscillator length $b = \sqrt{\hbar/m\omega} = 1/u$ the collective masses calculated in sect. 8 and 9 are

$$M(^{16}\text{O}) = 34m, \qquad (10.1)$$

$$M(^{40}\text{Ca}) = 120m. \qquad (10.2)$$

Therefore the classical energy function is

$$H(b, \dot{b}) = \frac{1}{2}M\dot{b}^2 + \mathscr{V}(b), \qquad (10.3)$$

where the collective potential energy can be identified with $B(\gamma)$ of eq. (8.6) if one puts $\gamma = 1/b$. Fig. 1 shows $\mathscr{V}(b)$ for ^{16}O and ^{40}Ca using the Skyrme II force (SkII). The actual calculations to be discussed below are performed with the interactions SkI, SkII and SkIII, the parameters of which can be found in refs. [9, 25]). All collective potentials show a very pronounced minimum around $b_0 = 1.72$ and 1.96 fm for ^{16}O and ^{40}Ca respectively. For small distances from the minimum they are well approximated by a parabola.

It is well known that there are ambiguities in quantizing a classical Hamiltonian. The Schrödinger equation corresponding to eq. (10.3) which we have solved is

$$\left[-\frac{\hbar^2}{2M} \frac{\mathrm{d}^2}{\mathrm{d}b^2} + \mathscr{V}(b) - E \right] \Psi(b) = 0. \qquad (10.4)$$

The boundary conditions are regularity of $\Psi(b)$ at $b \to 0$ and an exponential decrease

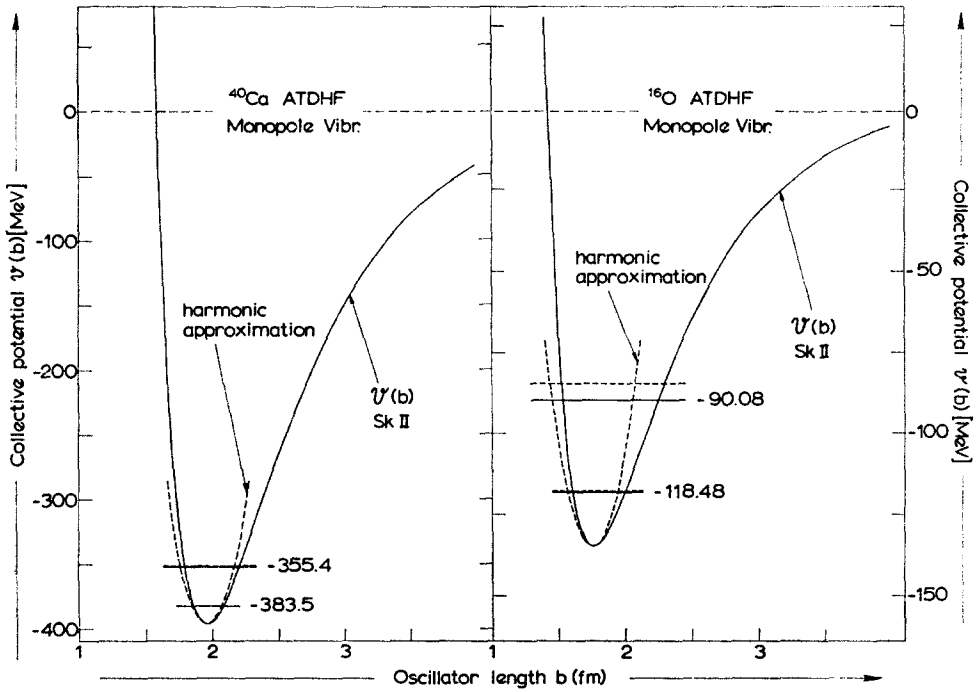Fig. 1. The collective potentials for the monopole vibrations in ^{16}O and ^{40}Ca calculated with the adiabatic time-dependent Hartree-Fock theory (ATDHF). Energy levels are given for the ground state and the first excited isoscalar breathing mode state. The dotted lines indicate the potential and energy levels obtained by the harmonic approximation.

at $b \to \infty$. The normalisation corresponding to (10.4) is

$$\int_0^\infty \mathrm{d}b\,|\Psi(b)|^2 = 1. \tag{10.5}$$

There is another possibility, namely to add the term $-(2/b)(\hbar^2/2M)\mathrm{d}/\mathrm{d}b$ to (10.4) and to use instead of $\mathrm{d}b$ the volume element $b^2\mathrm{d}b$. The ambiguity in quantizing eq. (10.3) may cause difficulties. However in the present case the $\Psi(b)$ of the low-lying excited states turn out to be sufficiently centred around the minimum of $\mathscr{V}(b)$, so that the difference in excitation energies of the first excited states comes out to be less than 0.1 MeV which is negligible compared to the absolute values of the excitation energies of more than 25 MeV.

Table 1 lists the excitation energies of the first isoscalar monopole vibration (isoscalar breathing mode) for ^{16}O and ^{40}Ca obtained with SkI, SkII and SkIII. The values are given for both the solution of the Schrödinger equation (10.4) and the harmonic approximation (8.17), denoted by E_{0^+} and $E_{0^+}^{\mathrm{harm}}$ respectively. All values show a decrease with increasing mass number as is qualitatively expected from the hydrodynamic model [24]. For both values, E_{0^+} as well as for $E_{0^+}^{\mathrm{harm}}$ the excitation

The excitation energies of the isoscalar monopole vibration in ^{16}O and ^{40}Ca, calculated with ATDHF

	^{16}O				^{40}Ca				
	K	$E_{0^+}^{harm}$	E_{0^+}	SZ	K	$E_{0^+}^{harm}$	E_{0^+}	SZ	BT
SkI	211.9	36.5	30.8		242.7	30.3	28.8		33.0
SkII	188.3	33.5	28.4	33.6	220.0	28.1	26.9	27.2	27.6
SkIII	196.3	34.0	28.9		228.6	28.6	27.2		

Presented are the compression modulus K (MeV), the excitation energy $E_{0^+}^{harm}$ (MeV) obtained with the harmonic approximation and the excitation energy E_{0^+} obtained by solving the Schrödinger equation. For comparison also the results of Sharp and Zamick [26]) and of Bertsch and Tsai [20]) are listed, denoted by SZ and BT respectively. All values are given for the three Skyrme interactions SkI, SkII and SkIII.

energies are rather independent on the particular parametrization of the Skyrme interaction used. This is due to the fact that ^{16}O and ^{40}Ca have rather harmonic potential energy surfaces around the minimum and also very similar compression moduli. However, the harmonic approximation turns out to be somewhat less justified for ^{16}O than for ^{40}Ca. But still the excitation energies agree within 15 %.

In table 1 some results of Sharp and Zamick [26]) and of Bertsch and Tsai [20]) are listed as well. Sharp and Zamick assume the breathing mode in ^{16}O as being generated by the electric monopole operator acting on the ground state, which is constructed from harmonic oscillator wave functions. Such a state would carry then all the strength of the monopole transition being a giant resonance in a strict sense. This is a simplified ansatz in the framework of a Tamm-Dancoff approximation and implies the assumption of a small amplitude. Therefore, one cannot expect more than a qualitative agreement.

Bertsch and Tsai [20]) describe the monopole vibrations by the RPA using Green function techniques in the coordinate space. The nuclear ground state is calculated fully self-consistently. Such an approach should correspond more to an ATDHF calculation using self-consistent single-particle energies.

Sharp and Zamick [26]) as well as Bertsch and Tsai [20]) make use of some sort of small amplitude approximation. Therefore, the agreement is expected to be best if one compares their values with ours calculated with the harmonic approach, $E_{0^+}^{harm}$. This is indeed the case as one can see in table 1.

11. Summary and conclusions

The explicit form of the time-dependent Hartree-Fock equations (TDHF) for Skyrme's interaction has been derived in coordinate space and the structure of the resulting equations has been discussed. We have demonstrated in particular that an important consequence of the equations of motion is the existence of a continuity equation. This equation holds for the total density but not for neutron and proton

densities separately because of the presence of exchange forces.

The limiting case of adiabatic motion (ATDHF), which is relevant to a large variety of problems in nuclear collective motion, has been investigated. We have shown that the equations of motion reduce in this case to a finite set of inhomogeneous linear differential equations. One significant accomplishment of these equations is that they avoid altogether the problem of finding a proper treatment of continuum states which is usually encountered in other approaches.

Applications of both TDHF and ATDHF to the description of isoscalar monopole vibrations have been considered for ^{16}O and ^{40}Ca, assuming the time-even part of the single-particle wave functions to be pure oscillator wave functions. In the case of the TDHF equation we have shown that, if the same assumption is made for time-odd components, then the equation of motion is analytically soluble and yields a collective Hamiltonian which is identical to the hydrodynamic result. In the case of ATDHF we have established that the equation for the collective mass can be solved exactly without further assumptions by using the continuity equation and generalised scaling properties of the single-particle wave functions. In case of monopole vibrations the result is again identical with the hydrodynamical formula, if one uses harmonic oscillator single-particle wave functions. A somewhat more realistic description of the breathing mode using constrained Hartree-Fock wave functions is presently under investigation.

Appendix A

THE HAMILTONIAN DENSITY

In this appendix we derive the Hamiltonian density for the Skyrme interaction. The derivation follows that given in appendices A and B of Vautherin and Brink [9]), except that we do not assume that the subspace of occupied states is invariant under time-reversal.

Referring to the previous definitions, eqs. (3.7) to (3.12), it is easily seen that the V_0 term, eq. (A.5) of Vautherin and Brink [9]) becomes

$$V_0 = \tfrac{1}{2}t_0 \int d^3r[(1+\tfrac{1}{2}x_0)\rho^2 -(x_0+\tfrac{1}{2})(\rho_p^2+\rho_n^2)+\tfrac{1}{2}x_0 s^2 -\tfrac{1}{2}(s_p^2+s_n^2)]. \qquad (A.1)$$

The V_1 term, (A.8), of ref. [9]) now contributes:

$$V_1 = -\tfrac{1}{16}t_1 \int d^3r \sum_{\substack{q_1 q_2 \\ \sigma_1\sigma'_1\sigma_2\sigma'_2}} [(1-\tfrac{1}{2}\delta_{q_1 q_2})\delta_{\sigma_1\sigma'_1}\delta_{\sigma_2\sigma'_2} -\tfrac{1}{2}\delta_{q_1 q_2}(\sigma'_1|\sigma_1|\sigma_1)\cdot(\sigma'_2|\sigma_2|\sigma_2)]$$
$$\times[(\nabla_1^2+\nabla_2^2-2\nabla_1\cdot\nabla_2+\nabla_1'^2+\nabla_2'^2-2\nabla_1'\cdot\nabla_2')$$
$$\times\rho_{q_1}(r_1\sigma_1,r_1'\sigma_1')\rho_{q_2}(r_2\sigma_2,r_2'\sigma_2')]_{r_1=r_1'=r_2=r_2'}. \qquad (A.2)$$

Consider first the direct term. Using the identities

$$[(\nabla^2 + \nabla'^2)\rho(r, r')]_{r=r'} = \nabla^2\rho(r) - 2\tau(r), \tag{A.3}$$

$$[\nabla\rho(r, r')]_{r=r'} = [\nabla'\rho(r, r')]^*_{r=r'} = \tfrac{1}{2}\nabla\rho(r) + ij(r). \tag{A.4}$$

We may write the direct contribution as

$$V_{1D} = -\tfrac{1}{16}t_1 \int d^3r \left[2\rho(\nabla^2\rho - 2\tau) - 2(\tfrac{1}{2}\nabla\rho + ij)^2 - 2(\tfrac{1}{2}\nabla\rho - ij)^2\right]$$

$$= -\tfrac{1}{16}t_1 \int d^3r (3\rho\nabla^2\rho - 4\rho\tau + 4j^2), \tag{A.5}$$

where, in proceeding to the last line we have performed an integration by parts. Making use of the additional identities,

$$[(\nabla^2 + \nabla'^2)s_\nu(r, r')]_{r=r'} = \nabla^2 s_\nu(r) - 2T_\nu(r), \tag{A.6}$$

$$[\nabla_\mu s_\nu(r, r')]_{r=r'} = [\nabla'_\mu s_\nu(r, r')]^*_{r=r'} = \tfrac{1}{2}\nabla_\mu s_\nu(r) + iJ_{\mu\nu}(r), \tag{A.7}$$

the exchange contribution may be written as

$$V_{1E} = -\tfrac{1}{16}t_1 \int d^3r \sum_q \{-\tfrac{3}{2}\rho_q \nabla^2\rho_q + 2\rho_q\tau_q - 2j_q^2 - s_q \cdot (\nabla^2 s_q - 2T_q)$$

$$+ \sum_{\mu\nu} [(\tfrac{1}{2}\nabla_\mu s_\nu + iJ_{\mu\nu})^2 + (\tfrac{1}{2}\nabla_\mu s_\nu - iJ_{\mu\nu})^2]\}$$

$$= -\tfrac{1}{16}t_1 \int d^3r \sum_q [-\tfrac{3}{2}\rho_q \nabla^2\rho_q + 2\rho_q\tau_q - 2j_q^2 - \tfrac{3}{2}s_q \cdot \nabla^2 s_q + 2s_q \cdot \overset{\leftrightarrow}{T}_q - 2\overset{\leftrightarrow}{J}_q^2]. \tag{A.8}$$

In this equation, $\overset{\leftrightarrow}{J}$ is the tensor of second rank with components $J_{\mu\nu}$; if $\overset{\leftrightarrow}{A}$ and $\overset{\leftrightarrow}{B}$ are tensors, their scalar product is defined by: $\overset{\leftrightarrow}{A} \cdot \overset{\leftrightarrow}{B} = \sum_{\mu\nu}A_{\mu\nu}B_{\mu\nu}$ in cartesian coordinates.

The calculation of the V_2 term proceeds quite similarly. Replacing $P_M P_\sigma P_\tau$ in ref. [9] eq. (A.16) by $-\tfrac{1}{2}(1 + \sigma_1 \cdot \sigma_2)\delta_{q_1 q_2}$, we have

$$V_2 = \tfrac{1}{4}t_2 \int d^3r_1 \sum_{\substack{q_1 q_2 \\ \sigma_1 \sigma'_1 \sigma_2 \sigma'_2}} [(1 + \tfrac{1}{2}\delta_{q_1 q_2})\delta_{\sigma_1 \sigma'_1}\delta_{\sigma_2 \sigma'_2} + \tfrac{1}{2}\delta_{q_1 q_2}\langle\sigma'_1|\sigma_1|\sigma_1\rangle\langle\sigma'_2|\sigma_2|\sigma_2\rangle$$

$$\times [(\nabla'_1 \cdot \nabla_1 - \nabla'_2 \cdot \nabla_1)\rho_{q_1}(r_1\sigma_1, r'_1\sigma'_1)\rho_{q_2}(r_2\sigma_2, r'_2\sigma'_2)]_{r_1 = r'_1 = r_2 = r'_2}. \tag{A.9}$$

Using eq. (A.4), the direct contribution may be written

$$V_{2D} = \tfrac{1}{4}t_2 \int d^3r [\rho\tau - (\tfrac{1}{2}\nabla\rho - ij)(\tfrac{1}{2}\nabla\rho + ij)] = \tfrac{1}{16}t_2 \int d^3r (4\rho\tau + \rho\nabla^2\rho - 4j^2). \tag{A.10}$$

Using, in addition, eq. (A.7), the exchange contribution follows as

$$
\begin{aligned}
V_{2E} &= \tfrac{1}{4}t_2 \int d^3r \sum_q \left[\tfrac{1}{2}\rho_q \tau_q - \tfrac{1}{2}(\tfrac{1}{2}\nabla\rho_q - ij_q)(\tfrac{1}{2}\nabla\rho_q + ij_q) + \tfrac{1}{2}s_q \cdot T_q \right.\\
&\quad \left. -\tfrac{1}{2}\sum_{\mu\nu}(\tfrac{1}{2}\nabla_\mu s_{q\nu} - iJ_{q,\mu\nu})(\tfrac{1}{2}\nabla_\mu s_{q\nu} + iJ_{q,\mu\nu}) \right]\\
&= \tfrac{1}{16}t_2 \int d^3r \sum_q (2\rho_q \tau_q + \tfrac{1}{2}\rho_q \nabla^2\rho_q - 2j_q^2 + 2s_q \cdot T_q + \tfrac{1}{2}s_q \cdot \nabla^2 s_q - 2\overset{\leftrightarrow}{J}_q^2).
\end{aligned} \tag{A.11}
$$

Our starting point for the calculation of the potential energy coming from the three-body force is (A.22), ref. [9]). Introducing the explicit form of the spin-exchange and charge-exchange operators we have

$$
\begin{aligned}
\tilde{V}_{123} &= t_3 \delta(r_1 - r_2)\delta(r_2 - r_3)[1 + \tfrac{1}{2}(1 + \sigma_1 \cdot \sigma_2 + \sigma_2 \cdot \sigma_3 + \sigma_1 \cdot \sigma_2 \sigma_2 \cdot \sigma_3)\delta_{q_1 q_2}\delta_{q_2 q_3} \\
&\qquad\qquad\qquad\qquad\qquad - \tfrac{3}{2}(1 + \sigma_1 \cdot \sigma_2)\delta_{q_1 q_2}] \\
&= t_3 \delta(r_1 - r_2)\delta(r_2 - r_3)[1 + \tfrac{1}{2}(1 + 3\sigma_1 \cdot \sigma_2 - i\sigma_1 \cdot \sigma_2 \times \sigma_3)\delta_{q_1 q_2}\delta_{q_2 q_3} \\
&\qquad\qquad\qquad\qquad\qquad - \tfrac{3}{2}(1 + \sigma_1 \cdot \sigma_2)\delta_{q_1 q_2}],
\end{aligned} \tag{A.12}
$$

where, in proceeding to the last line, we have made use of the identity $\sigma_1 \cdot \sigma_2 \sigma_2 \cdot \sigma_3 = \sigma_1 \cdot \sigma_3 - i\sigma_1 \cdot (\sigma_2 \times \sigma_3)$, and of the symmetry of the integrand to relabel the particles. Substituting eq. (A.12) into ref. [9]) eq. (A.20) we find the three-body contribution

$$
\begin{aligned}
V_3 &= \tfrac{1}{6}t_3 \int d^3r \left[\rho^3 + \tfrac{1}{2}(\rho_p^3 + \rho_n^3) + \tfrac{3}{2}(\rho_p s_p^2 + \rho_n s_n^2) - \tfrac{3}{2}\rho(\rho_p^2 + \rho_n^2) - \tfrac{3}{2}\rho(s_p^2 + s_n^2) \right] \\
&= \tfrac{1}{4}t_3 \int d^3r \left[\rho_p(\rho_n^2 - s_n^2) + \rho_n(\rho_p^2 - s_p^2) \right].
\end{aligned} \tag{A.13}
$$

(The term $i\sigma_1 \cdot (\sigma_2 \times \sigma_3) \rightarrow s_q \cdot (s_q \times s_q) = 0$.)

The spin-orbit contribution to the potential energy is obtained by substituting (B.3) into (B.2) (both of them are of ref. [9])):

$$
\begin{aligned}
E_{s.o.} &= \tfrac{1}{4}iV_{s.o.} \sum_{q_1 q_2}(1 + \delta_{q_1 q_2}) \int d^3r_1 \sum_{\lambda\mu\nu} \varepsilon_{\lambda\mu\nu}[\nabla'_{1\lambda}\nabla_{1\mu}\rho_{q_1}(r_1, r'_1)s_{q\nu}(r_2, r'_2) \\
&\quad + (\nabla'_{1\lambda}\nabla_{1\mu} - \nabla'_{1\lambda}\nabla_{2\mu} - \nabla'_{2\lambda}\nabla_{1\mu})s_{q\nu}(r_1, r'_1)\rho_{q_2}(r_2, r'_2)]_{r_1 = r'_1 = r_2 = r'_2}.
\end{aligned} \tag{A.14}
$$

Using eqs. (A.4) and (A.7) we may rewrite eq. (A.14)

$$
\begin{aligned}
E_{s.o.} &= \tfrac{1}{4}iV_{s.o.} \sum_{q_1 q_2}(1 + \delta_{q_1 q_2}) \int d^3r_1 \{ \nabla'_1 \times \nabla_1 \rho_{q_1}(r_1, r'_1) \cdot s_{q_2}(r_2) + \nabla'_1 \cdot \nabla_1 \times s_{q_1}(r_1, r'_1) \\
&\quad -\sum_{\mu\nu\lambda} \varepsilon_{\lambda\mu\nu}[(\tfrac{1}{2}\nabla_{1\lambda}s_{q_2\nu}(r_1) - iJ_{q_2,\mu\nu}(r))(\tfrac{1}{2}\nabla_{1\mu}\rho_{q_1}(r_1) + ij_{q_1\mu}(r_1)) \\
&\quad + (\tfrac{1}{2}\nabla_{1\lambda}\rho_{q_2}(r_1) - ij_{q_2\lambda}(r_1))(\tfrac{1}{2}\nabla_{1\mu}s_{q_1\nu}(r_1) + iJ_{q,\mu\nu}(r_1))]\}_{r_1 = r'_1 = r_2} \\
&= \tfrac{1}{4}iV_{s.o.} \sum_{q_1, q_2}(1 + \delta_{q_1 q_2}) \int d^3r_1 \{ [\nabla'_1 \times \nabla_1 \rho_{q_1}(r_1, r'_1)]_{r_1 = r'_1} s_{q_2\nu}(r_1) \\
&\quad + [\nabla'_1 \cdot \nabla_1 \times s_q(r_1, r'_1)]_{r_1 = r'_1}\rho_{q_2}(r_1) - i\sum_{\lambda\mu\nu} \varepsilon_{\lambda\mu\nu}[\nabla_{1\lambda}s_{q_2\nu}(r_1)j_{q,\mu}(r_1) \\
&\qquad\qquad\qquad\qquad\qquad\qquad - J_{q_2,\lambda\nu}(r_1)\nabla_{1\mu}\rho_{q_1}(r_1)]\}.
\end{aligned} \tag{A.15}
$$

Using the identities

$$[(\nabla' \times \nabla)\rho(r, r')]_{r=r'} = i\nabla \times j(r), \tag{A.16}$$

$$[\nabla' \cdot \nabla s(r, r')] = i\sum_{\mu\nu\lambda}\varepsilon_{\lambda\mu\nu}\nabla_\lambda J_{\mu\nu} = i\overleftrightarrow{\nabla}\cdot\overleftrightarrow{J}, \tag{A.17}$$

where the components of $\overleftrightarrow{\nabla}$ is defined by $\nabla_{\mu\nu} = \sum_\lambda\varepsilon_{\mu\nu\lambda}\nabla_\lambda$, we may, after integration by parts, write

$$E_{\text{s.o.}} = -\tfrac{1}{2}V_{\text{s.o.}}\sum_{qq'}(1+\delta_{qq'})\int d^3r\,[(\nabla\times j_q)\cdot s_{q'}+\rho_{q'}\overleftrightarrow{\nabla}\cdot\overleftrightarrow{J}_q]. \tag{A.18}$$

The term $\int d^3r(\nabla\times j)\cdot s$ appearing in (A.18) can also be written as $\int d^3r\,j\cdot(\nabla\times s)$ in view of the vector identity

$$\nabla\cdot(A\times B) = B\cdot\nabla\times A - A\cdot\nabla\times B.$$

This expression will also be needed in the derivation of the HF Hamiltonian in appendix B.

The Hamiltonian density is obtained by adding the kinetic energy density $(\hbar^2/2m)\tau(r)$ and the integrands of eqs. (A.1), (A.5), (A.8), (A.10), (A.11), (A.13) and (A.15) with the result:

$$H(r) = \frac{\hbar^2}{2m}\tau + \tfrac{1}{2}t_0[(1+\tfrac{1}{2}x_0)\rho^2 - (x_0+\tfrac{1}{2})(\rho_p^2+\rho_n^2) + \tfrac{1}{2}x_0 s^2 - \tfrac{1}{2}(s_p^2+s_n^2)]$$

$$+ \tfrac{1}{4}(t_1+t_2)(\rho\tau - j^2) + \tfrac{1}{16}(t_2-3t_1)\rho\nabla^2\rho + \tfrac{1}{32}(t_2+3t_1)\sum_q(\rho_q\nabla^2\rho_q + s_q\nabla^2 s_q)$$

$$+ \tfrac{1}{8}(t_2-t_1)\sum_q[\rho_q\tau_q - j_q^2 + s_q\cdot T_q - \overleftrightarrow{J}_q^2] - \tfrac{1}{2}V_{\text{s.o.}}\sum_{qq'}(1+\delta_{qq'})[s_q\cdot\nabla\times j_{q'} + \rho_q\overleftrightarrow{\nabla}\cdot\overleftrightarrow{J}]$$

$$+ H_C(r). \tag{A.19}$$

In this equation $H_C(r)$ is the Coulomb energy density, (see eq. (13) of ref. [9]). The various densities are defined in eqs. (3.7)–(3.12). Eq. (4.4) can be compared with eq. (12) of ref. [9]. There, only the antisymmetric part of $J_{\mu\nu}$ was retained in the spin-orbit density $J(r)$. Apart from the momentum current j also the spin density s and the vector part of the kinetic energy density T (in (A.19)) are new compared to static HF. Notice that the momentum density j and the spin current tensor $\overleftrightarrow{J}_{\mu\nu}$ occur in the combination $\rho\tau-j^2$ and $s\cdot T - J^2$ respectively. As discussed in sect. 4, this feature reflects the Galilean invariance of the Skyrme interaction.

Appendix B

THE HARTREE-FOCK HAMILTONIAN

From eq. (A.19) the binding energy difference, eq. (2.3), can be written as

$$\delta E = \sum_q\int d^3r\left\{\frac{\hbar^2}{2m_q^*(r)}\delta\tau_q(r) + U_q(r)\delta\rho_q(r) + \overleftrightarrow{B}_q(r)\cdot\overleftrightarrow{\delta J}_q(r) + I_q(r)\cdot\delta j_q(r)\right.$$

$$\left. + C_q(r)\cdot\delta T_q(r) + \Sigma_q(r)\delta s_q(r), \tag{B.1}\right.$$

where

$$\frac{\hbar^2}{2m_q^*(r)} = \frac{\hbar^2}{2m} + \tfrac{1}{4}(t_1+t_2)\rho + \tfrac{1}{8}(t_2-t_1)\rho_q,$$ (B.2)

$$U_q(r) = t_0[(1+\tfrac{1}{2}x_0)\rho - (x_0+\tfrac{1}{2})\rho_q] + \tfrac{1}{8}(t_2-3t_1)\nabla^2\rho + \tfrac{1}{16}(3t_1+t_2)\nabla^2\rho_q$$

$$+ \tfrac{1}{4}(t_1+t_2)\tau + \tfrac{1}{8}(t_2-t_1)\tau_q + \tfrac{1}{4}t_3(\rho^2-\rho_q^2-(s-s_q)^2) - \tfrac{1}{2}V_{s.o.}\overset{\leftrightarrow}{\nabla}\cdot(\overset{\leftrightarrow}{J}+\overset{\leftrightarrow}{J}_q),$$ (B.3)

$$\overset{\leftrightarrow}{B}_q = -\tfrac{1}{4}(t_2-t_1)\overset{\leftrightarrow}{J}_q + \tfrac{1}{2}V_{s.o}\overset{\leftrightarrow}{\nabla}(\rho+\rho_q),$$ (B.4)

$$I_q(r) = -\tfrac{1}{2}(t_1+t_2)j - \tfrac{1}{4}(t_2-t_1)j_q - \tfrac{1}{2}V_{s.o.}\nabla\times(s+s_q),$$ (B.5)

$$C_q(r) = \tfrac{1}{8}(t_2-t_1)s_q,$$ (B.6)

$$\Sigma_q(r) = \tfrac{1}{2}t_0(x_0s-s_q) + \tfrac{1}{8}(t_2-t_1)T_q + \tfrac{1}{16}(t_2+3t_1)\nabla^2 s_q - \tfrac{1}{2}t_3(\rho-\rho_q)s_q - \tfrac{1}{2}V_{s.o.}\nabla\times(j+j_q).$$

(B.7)

Since the complete derivation of the Hartree-Fock Hamiltonian is elementary but rather lengthy, we consider in detail only the $j\cdot\delta j$ term contained in (B.1) as an example:

$$\delta j = \frac{1}{2i}\sum_{k\sigma}[\delta\Phi_k^*(r\sigma)\nabla\Phi_k(r\sigma) + \Phi_k^*(r\sigma)\nabla\delta\Phi_k(r\sigma) - (\nabla\delta\Phi_k(r\sigma))^*\Phi_k(r\sigma)$$

$$- (\nabla\phi(r\sigma))^*\delta\Phi_k(r\sigma)]. \quad \text{(B.8)}$$

Integration by parts gives

$$j\cdot\delta j = \frac{1}{2i}\sum_{k\sigma}[\delta\Phi_k^*(r\sigma)(\nabla\cdot j + j\cdot\nabla)\Phi_k(r\sigma) - \delta\Phi_k(r\sigma)(\nabla\cdot j + j\cdot\nabla)\Phi_k^*(r\sigma)].$$ (B.9)

Therefore the contribution of this term to the HF fields is

$$j\cdot\delta j \rightarrow \frac{1}{2i}(\nabla\cdot j + j\cdot\nabla).$$ (B.10)

In a similar way it can be shown that

$$\rho\delta\tau \rightarrow -\nabla\cdot\rho\nabla,$$ (B.11)

$$s\cdot\delta T \rightarrow -\sum_{\mu\nu}\sigma_\nu\nabla_\mu s_\nu\nabla_\mu,$$ (B.12)

$$\overset{\leftrightarrow}{J}\cdot\overset{\leftrightarrow}{\delta J} \rightarrow \frac{1}{2i}\sum_{\mu\nu}\sigma_\nu(\nabla_\mu J_{\mu\nu}+J_{\mu\nu}\nabla_\mu),$$ (B.13)

$$\delta\rho \rightarrow 1,$$ (B.14)

$$\delta s_\nu \rightarrow \sigma_\nu.$$ (B.15)

Collecting the time-even quantities, we obtain

$$W_+^{(q)}(r) = -\nabla\cdot\frac{\hbar^2}{2m_q^*(r)}\nabla + U_q + \frac{1}{2i}(\overset{\leftrightarrow}{\nabla\sigma}\cdot\overset{\leftrightarrow}{B}_q + \overset{\leftrightarrow}{B}_q\cdot\overset{\leftrightarrow}{\nabla\sigma}),$$ (B.16)

where $\overset{\leftrightarrow}{\nabla\sigma}$ is the tensor whose components are $\nabla_\mu\sigma_\nu$. Collecting the time-odd quantities, we find

$$W_-^{(q)}(r) = -\nabla \cdot (\sigma \cdot C_q)\nabla + \sigma \cdot \Sigma_q + \frac{1}{2i}(\nabla \cdot I_q + I_q \cdot \nabla). \qquad (B.17)$$

In eqs. (B.9)–(B.17) the ∇-operator acts on all functions on its right hand side, including the wave function Φ e.g. $\nabla \cdot j\Phi = (\nabla \cdot j)\Phi + j \cdot \nabla\Phi$. For TDHF the total HF Hamiltonian is just

$$W^{(q)} = W_+^{(q)} + W_-^{(q)}. \qquad (B.18)$$

For ATDHF one can identify $W_0^{(q)}$ with $W_+^{(q)}$, provided ρ is replaced by ρ_0. However, one should omit in U_q the term proportional to $(s - s_q)^2$ since it originates from ρ_1 and is, therefore, of second order in χ. $W_1^{(q)}$ can be identified with $W_-^{(q)}$ provided one calculates the time-odd densities from ρ_1 obtained by solving the ATDHF equations (6.8).

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