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Static Hartree-Fock Calculations using the Imaginary Time Step Method

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ABSTRACT

Static Hartree-Fock Calculations using the Imaginary Time Step Method

Daniel Provost

Static Hartree-Fock calculations using the Skyrme's density-dependent effective nucleon-nucleon interaction are performed by the imaginary time step method. The Time-Dependent Hartree-Fock method is discussed in detail. Axially symmetric calculations have been made for the closed-shell nucleus ^{40}Ca.

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INTRODUCTION

In spite of the relatively strong nucleon-nucleon interaction, a description of the nucleus as being a set of noninteracting nucleons moving in a common potential provides a reasonable approximation to nuclear properties. The nuclear forces and the Pauli exclusion principle act together so as to provide this common potential well. The question is how to obtain such a single-particle potential.

The Hartree-Fock method provides a tool for calculating the common potential from an effective nucleon-nucleon interaction. Using a density-dependent effective interaction such as Skyrme's interaction, static Hartree-Fock calculations are able to reproduce the ground state properties of sherical nuclei very well.

A natural assumption is that the independent-particle picture can also be applied to the dynamics of nuclear systems. The Time-Dependent Hartree-Fock method is based upon this assumption. It was found recently that the Time-Dependent Hartree-Fock (TDHF) method could describe reasonably well many low energy phenomena.

It was also found recently that by using a small imaginary time step in the TDHF equations, the resulting wave functions would converge to the static Hartree-Fock (HF) solutions. We develop a computer program that will perform axially symmetric TDHF calculations. We then perform static HF calculations for ^{40}Ca using the imaginary time step method.

In Chapter 2 we discuss in detail the TDHF method. Chapter 3 deals with Skyrme's interaction and the resulting energy functional. The calculational details are presented in Chapter 4. The results and discussion are presented in Chapter 5. Chapter 6 contains the concluding remarks.

Chapter 1

THE MOTIVATION FOR THE HARTREE-FOCK METHOD

The microscopic description of a nucleus comprising of A nucleons is a quantum many-body problem. Describing the nucleus by the wave function $\Psi(t)$, Schrodinger's equation governs the dynamics of the A nucleons:

$$H \Psi(t) = i\hbar \frac{\partial}{\partial t} \Psi \quad . \tag{1.1}$$

where H is the full many-body Hamiltonian of the system. This 3A-dimensional linear equation is solvable only in very special cases. Some approximations must therefore be used to simplify Eq. 1.1.

In spite of the relatively strong nucleon-nucleon interaction, the description of the nucleus as being a set of noninteracting nucleons moving in a common potential provides a reasonable approximation to nuclear properties. The nuclear forces and the Pauli exclusion principle act together so as to provide this common potential well. The question is how to obtain such a potential and stay true to the properties of the full many-body Hamiltonian H . We also need that certain physical laws remain unchanged. Conservation of the mass number, total linear momentum and total angular momentum must hold. Furthermore, the total wave function must represent a system of A fermions - the total wave function must be anti-symmetrized with respect to the exchange of nucleons.

The static Hartree-Fock (HF) method and its dynamical counterpart, the Time-Dependent Hartree-Fock (TDHF) method satisfy these requirements. These methods calculate the above mentioned common potential from a given nucleon-nucleon interaction and reduces Eq. 1.1 to A 3-dimensional coupled nonlinear equations. We now turn our attention to the nucleon-

nucleon interaction. Bare nucleon-nucleon forces have an infinite or at least a very repulsive core. The two-body matrix elements entering the Hartree-Fock potential all become infinite for a hard core potential. This prevents the direct application of the Hartree-Fock method with the fundamental bare nucleon-nucleon interactions. This problem can be solved by replacing the bare nucleon-nucleon interaction with a consistent resummation of certain higher order terms of the full many-body Hamiltonian as is done in Bruckner theory[61,63]. The resulting Bruckner G-matrix solves the hard-core problem. Bruckner Hartree-Fock calculations turned out to be quite deceiving. Although the nuclear radii for several nuclei were reproduced, the corresponding binding energies were grossly underestimated. Negele and Vautherin[37] proposed the Local Density Approximation for the nucleon-nucleon interaction. As in the Bruckner theory, the nucleon-nucleon interaction is replaced by the G-matrix. However now the nuclear G-matrix is calculated at each point as if the nucleus around that point were a piece of nuclear matter. The solution of the resulting HF equations is very complicated because a set of coupled integro-differential equations need to be solved. A further approximation can be made by noting that the nuclear force is short-ranged. The nonlocal exchange term in the HF equations can be expanded in powers of the nonlocality around its local value. This leads us in a quite natural way to the phenomenological Skyrme nucleon-nucleon interaction which is to be used in the calculations presented here. Static HF calculations can reproduce remarkably well the ground state properties of doubly-closed shell nuclei[28,36]. TDHF calculations have also had tremendous success using this interaction (see section 2.1).

Chapter 2

THE TIME DEPENDENT HARTREE-FOCK METHOD (TDHF)

2.1 Introduction

A complete microscopic description of large amplitude motions in nuclei, such as anharmonic vibrations or fission and fusion processes, is not feasible at the present time. However, there exists a need for a microscopic theory that would be able to describe the general nuclear properties and the dynamics starting from a nucleon-nucleon interaction. This would be in constrast with the multitude of models which have phenomenologically built into them just those properties one wishes to reproduce. Only certain degrees of freedom are included in these models and when another phenomena is examined, new models are invoked, thereby losing any possibility for a general unified description. Understanding the shortcomings of such models enables one to be tolerant of the numerical difficulties associated with solving the equations arising from microscopic theories.

One method for treating microscopically nuclear reactions that merits serious consideration is a direct solution of the TDHF equations, which were first proposed by Dirac in 1930[1]. The fundamental physical assumption is that the independent particle aspects of near-equilibrium nuclear states persist to highly non-equilibrium situations. Following the first schematic applications of the TDHF method to large amplitude nuclear dynamics[2-5], numerous calculations have appeared: Fission (Refs. 18,52), heavy-ion fusion (Refs. 6,7,11,12,14,18-20,22,23,25,26,27, 85,86), and deep-inelastic collisions (Refs. 6-11,13,15-17,19-21,24,25,33, 85,86,87) calculations have had varying degrees of qualitative and quantitative success.

In this chapter we shall examine the theory behind the TDHF method. In section 2.2 we derive the TDHF equations and examine the immediate physical consequences. In section 2.3 a variational derivation of the TDHF equations is presented. Section 2.4 examines the properties of the TDHF equations, and in section 2.5 there is a general discussion of the TDHF method.

2.2 The TDHF Equations

The description of the nucleus in terms of a non-dispersive wave packet is very close to our classical intuition. For instance, in the fission process we physically picture a nucleus as a liquid drop which at each instant in time has a fixed deformation. Microscopically, such a state can be represented by a single Slater determinant in a deformed potential well which can be used to approximate the full many-body Hamiltonian. This type of wave packet will be seen to satisfy the TDHF equations.

We therefore consider an arbitrary wave packet $|\Psi(0)\rangle$. Its time evolution is given for all time by the equation

$$|\Psi(t)\rangle = e^{-iHt/\hbar}\,|\Psi(0)\rangle \tag{2.1}$$

where H is the full many-body Hamiltonian. The wave function $|\Psi(t)\rangle$ is, in principle, equivalent to the solution of the stationary Schrodinger equation. The one-body density at time t for the arbitrary wave packet is given by

$$\rho_{\alpha\beta}(t) = \langle \Psi(t)|\, C_\beta^\dagger C_\alpha \,|\Psi(t)\rangle \tag{2.2}$$

where the subscript labels refer to a complete set of single-particle states describing spatial, spin, and isospin nucleon coordinates. The annihilation and creation operators satisfy the usual fermion anti-commutation rules

$$\begin{aligned} \{C^+_\alpha, C^+_\beta\} = \{C_\alpha, C_\beta\} = 0 \\ \{C^+_\alpha, C_\beta\} = \delta_{\alpha\beta} \end{aligned} \tag{2.3}$$

The time derivative of Eq. 2.2 leads to the equation of motion of the one-body density

$$i\hbar\dot{\rho}_{\alpha\beta}(t) = \langle \Psi(t)|[C^+_\beta C_\alpha, H]|\Psi(t)\rangle \tag{2.4}$$

If the A nucleons interact with each other through a non-singular gallilean-invariant two-body interaction $v(\vec{r}', \vec{r})$, the many-body Hamiltonian in second-quantized notation is

$$H = \sum_{\alpha\beta} t_{\alpha\beta} C^+_\alpha C_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta,\gamma\delta} C^+_\alpha C^+_\beta C_\delta C_\gamma \tag{2.5}$$

where the matrix elements of the one-body kinetic energy are

$$t_{\alpha\beta} = \langle\alpha|t|\beta\rangle \tag{2.6}$$

and those of the anti-symmetrized two-body interaction are

$$\bar{v}_{\alpha\beta,\gamma\delta} = \langle\alpha\beta|v|\gamma\delta - \delta\gamma\rangle \tag{2.7}$$

with this Hamiltonian, Eq. 2.4 becomes

$$i\hbar\dot{\rho}_{\alpha\beta} - \sum_{\gamma}(t_{\alpha\gamma}\rho_{\gamma\beta} - \rho_{\alpha\gamma}t_{\gamma\beta}) = \frac{1}{2}\sum_{\gamma\delta\mu}\Big(\bar{v}_{\alpha\gamma,\delta\mu}\,\rho^{(2)}_{\delta\mu\beta\gamma} - \bar{v}_{\delta\mu,\beta\gamma}\,\rho^{(2)}_{\alpha\gamma\delta\mu}\Big) \tag{2.8}$$

where the two-body density matrix $\rho^{(2)}$ is defined by

$$\rho^{(2)}_{\alpha\beta\gamma\delta}(t) = \langle\Psi(t)|C^{+}_{\gamma}C^{+}_{\delta}C_{\beta}C_{\alpha}|\Psi(t)\rangle \tag{2.9}$$

The time evolution of ρ is hence related to the two-body density $\rho^{(2)}$. The time evolution of $\rho^{(2)}$ in turn can easily be shown to depend on the three-body density $\rho^{(3)}$, and so on. This ordered structure terminates at $\rho^{(A)}$ which is equivalent to solving the exact Schrodinger equation. The left hand side of Eq. 2.8 would describe the motion of the system if it were free ($v(\vec{r}',\vec{r})=0$). The right hand side of Eq. 2.8 contains the interaction between the particles and this interaction can be broken up into two parts:

(1) in a self-consistent one-body field.

(2) in individual collisions between the nucleons which cannot be accounted for by the mean field.

The latter is the cause of the two-body correlations.

To extract the two-body correlations required by the Pauli exclusion principle, we express the two-body density $\rho^{(2)}$ as an antisymmetrized product of two one-body density matrices and a correlation function $g^{(2)}$ which cannot be decomposed into products of one-body densities:

$$\rho^{(2)}_{\alpha\beta\gamma\delta} = \rho_{\alpha\gamma}\rho_{\beta\delta} - \rho_{\alpha\delta}\rho_{\beta\gamma} + g^{(2)}_{\alpha\beta\gamma\delta} \tag{2.10}$$

Equation 2.8 becomes

$$i\hbar\dot{\rho}_{\alpha\beta} - [t+\Gamma,\rho]_{\alpha\beta} = \frac{1}{2}\sum_{\gamma\delta\mu}\left(\bar{v}_{\alpha\gamma,\delta\mu}\, g^{(2)}_{\delta\mu\beta\gamma} - \bar{v}_{\delta\mu,\beta\gamma}\, g^{(2)}_{\alpha\gamma\delta\mu}\right) \tag{2.11}$$

with the density dependent Hartree-Fock potential

$$\Gamma_{\alpha\beta} = \sum_{\gamma\delta}\bar{v}_{\alpha\delta,\beta\gamma}\,\rho_{\gamma\delta} \tag{2.12}$$

It can be seen from Eq. 2.11 that the particles in this system can undergo two kinds of reactions:

(1) collisions with the moving walls of the mean field Γ causing "one-body friction"

(2) collisions with other particles causing "two-body friction".

Assuming that the two-body collisions can be neglected when the excitation energy per particle is less than the Fermi energy (as is done in the static case), Eq. 2.11 becomes

$$i\hbar\dot{\rho} = [h,\rho] \tag{2.13}$$

with $h = t + \Gamma$. Equation 2.13 is one form of the TDHF equations first formulated by Dirac in 1930[1].

Hence in the mean-field approximation, single-particle wave functions move inside the nucleus as free wave packets in a time-dependent potential. Energy dissipation and the time evolution of the nuclear surface arise from scattering on the edges of the self-consistent potential Γ.

A more useful form for the TDHF equations can be obtained by noting that the two-body density $\rho^{(2)}$ factorizes into uncorrelated pairs of the one-body density when the correlation function $g^{(2)}$ is set to zero:

$$\rho^{(2)}_{\alpha\beta\gamma\delta} = \rho_{\alpha\gamma}\rho_{\beta\delta} - \rho_{\alpha\delta}\rho_{\beta\gamma} \tag{2.14}$$

Setting $\beta = \delta$ in Eq. 2.14 and summing over this index, we get

$$\sum_{\beta} \rho^{(2)}_{\alpha\beta\gamma\beta} = A\rho_{\alpha\gamma} - (\rho^{2})_{\alpha\gamma} \tag{2.15}$$

Moreover, from the definition of $\rho^{(2)}$ (Eq. 2.9),

$$\sum_{\beta} \rho^{(2)}_{\alpha\beta\gamma\beta} = (A-1)\rho_{\alpha\gamma} \tag{2.16}$$

Combining Eqs. 2.15 and 2.16 we get the important result

$$\rho^{2} = \rho \tag{2.17}$$

Hence ρ is a projector and has eigenvalues 0 and 1. Further, since the trace of ρ is A, precisely A of the eigenvalues are 1. The one-body density ρ may therefore be written in a spectral expansion

$$\rho_{\alpha\beta} = \sum_{i=1}^{A} \psi_i(\alpha)\psi_i^{*}(\beta) \tag{2.18}$$

where the A single-particle wave functions $\psi_i(\alpha)$ span the space of unit eigenvalues:

$$\sum_{\alpha} \rho_{\alpha\beta}\, \psi_i(\alpha) = \psi_i(\beta) \qquad (2.19)$$

and are orthonormal:

$$\sum_{\alpha} \psi_j^{*}(\alpha)\, \psi_k(\alpha) = \delta_{jk} \qquad (2.20)$$

Equation 2.18 is consistent with a determinental many-body wave function

$$\Psi_{S.D.}(t) = \frac{1}{\sqrt{A!}} \det \left\{ \psi_1(t)\, \psi_2(t) \ldots\ldots \psi_A(t) \right\} \qquad (2.21)$$

where each single-particle wave function satisfies the TDHF equation:

$$i\hbar \frac{\partial}{\partial t} \psi_i(\alpha) = \sum_{\beta} h_{\alpha\beta}(t)\, \psi_i(\beta) \qquad (2.22)$$

We note that the original 3A-dimensional linear Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi = H \Psi \qquad (2.23)$$

is replaced by A coupled, non-linear 3-dimensional equations.

The representation of the TDHF equations (Eq. 2.22) in coordinate space is, for a spin independent two-body potential,

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \psi_i(\vec{r},t) = {} & \left(-\frac{\hbar^2}{2m} \nabla^2 + \Gamma_H(\vec{r},t) \right) \psi_i(\vec{r},t) \\ & + \int d\vec{r}\,'\, \Gamma_{ex}(\vec{r},\vec{r}\,',t)\, \psi_i(\vec{r}\,',t) \end{aligned} \qquad (2.24)$$

where the local H.F. potential is

$$\Gamma_H(\vec{r},t) = \int d\vec{r}\,'\, v(\vec{r},\vec{r}\,')\, \rho(\vec{r}\,',t) \qquad (2.25)$$

and the nonlocal, or exchange potential is

$$\Gamma_{ex}(\vec{r},\vec{r}',t) = -v(\vec{r},\vec{r}')\rho(\vec{r},\vec{r}',t) \tag{2.26}$$

In coordinate space, the one-body density has the form

$$\rho(\vec{r},\vec{r}',t) = \sum_{i=1}^{A} \psi_i(\vec{r},t)\,\psi_i^*(\vec{r}',t) \tag{2.27}$$

Most of the physics imbedded in the TDHF equations appear in Eq. 2.24. Each single-particle wave function evolves in a mean-field which is generated by the instantaneous configuration of all the nucleons, and it is only this mean field that couples the wave functions.

2.3 Variational Derivation of the TDHF equations

A variational derivation of the TDHF equations[34,48] provides further physical insights. The full many-body Schrodinger equation follows from the independent variations of the action

$$S = \int dt \,\langle \Psi(\vec{r}_1,\ldots,\vec{r}_A,t)|\, i\hbar\frac{\partial}{\partial t} - H\,|\Psi(\vec{r}_1,\ldots,\vec{r}_A,t)\rangle \tag{2.28}$$

with respect to $\psi_i(\vec{r},t)$ and its complex conjugate $\psi_i^*(\vec{r},t)$. To obtain the TDHF equations, we restrict the wave function to a single time-dependent Slater determinant:

$$\Psi_{SD}(\vec{r}_1,\ldots,\vec{r}_A,t) = \frac{1}{\sqrt{A!}}\det\left\{\psi_1(\vec{r}_1,t)\ldots\ldots\psi_A(\vec{r}_A,t)\right\} \tag{2.29}$$

where the single-particle wave functions are taken to be orthonormal. The action S becomes

$$\mathcal{S} = \int dt \left[\sum_{\alpha} \int d\vec{r}\, \psi^*_{\alpha}(\vec{r})\, i\hbar \frac{\partial}{\partial t} \psi_{\alpha}(\vec{r}) - \mathcal{H}(\psi^*, \psi) \right] \tag{2.30}$$

where

$$\begin{aligned} \mathcal{H}(\psi^*,\psi) = {} & \sum_{\alpha} \int d\vec{r}\, \psi^*_{\alpha}(\vec{r})\, t(\vec{r})\, \psi_{\alpha}(\vec{r}) \\ & + \frac{1}{2} \sum_{\alpha\beta} \int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3\, d\vec{r}_4\, \psi^*_{\alpha}(\vec{r}_1)\, \psi^*_{\beta}(\vec{r}_2) \\ & \cdot \tilde{V}(\vec{r}_1, \vec{r}_2; \vec{r}_3, \vec{r}_4)\, \psi_{\beta}(\vec{r}_4)\, \psi_{\alpha}(\vec{r}_3) \end{aligned} \tag{2.31}$$

The anti-symmetrized potential has the form

$$\tilde{V}(\vec{r}_1, \vec{r}_2; \vec{r}_3, \vec{r}_4) = \langle \vec{r}_1\, \vec{r}_2 \,|\, v \,|\, \vec{r}_3 \vec{r}_4 - \vec{r}_4 \vec{r}_3 \rangle \tag{2.32}$$

and the kinetic energy operator is denoted by $t(\vec{r})$. Euler's equation takes the form

$$i\hbar \frac{\partial}{\partial t} \psi_{\alpha}(\vec{r}) = \frac{\partial \mathcal{H}}{\partial \psi^*_{\alpha}(\vec{r})} \tag{2.33}$$

for a variation with respect to ψ^*_{α} and similarly

$$-i\hbar \frac{\partial}{\partial t} \psi^*_{\alpha}(\vec{r}) = \frac{\partial \mathcal{H}}{\partial \psi_{\alpha}(\vec{r})} \tag{2.34}$$

for a variation with respect to ψ_{α}. Eqs. 2.33 and 2.34 are another form of the TDHF equations. For a spin-independent two-body potential $v(\vec{r}, \vec{r}\,')$, Eq. 2.33 is easily seen to transform into Eq. 2.24.

The TDHF approximation thus acquires the form of a classical field theory, with the Hamiltonian $\mathcal{H}(\psi^*, \psi)$ given in Eq. 2.31 obeying the Hamiltonian equation 2.33 and its complex conjugate. Since any unitary transformations among the ψ_α's yield the same determinant (Eq. 2.29), the field theory is correspondingly gauge invariant with respect to these unitary transformations. Moreover, the TDHF equations can be regarded as describing the time evolution of a single Slater determinantal wave function which minimizes the expectation value of the many-body Schrodinger equation.

2.4 Properties of the TDHF Equations

2.4.1 Conservation of Orthonormality

The single-particle wave functions $\psi_i(\vec{r},t)$ stay orthonormal for all times:

$$i\hbar \frac{\partial}{\partial t} \langle \psi_i | \psi_k \rangle = \langle \psi_i | h - h^+ | \psi_k \rangle = 0 \tag{2.35}$$

since h is hermitian.

2.4.2 Conservation of Product Character

Starting at time t_0 with $\rho^2(t_0) = \rho(t_0)$, then at any later time, $\rho^2(t) = \rho(t)$:

$$i\hbar \frac{\partial}{\partial t} (\rho^2 - \rho) = i\hbar(\dot{\rho}\rho + \rho\dot{\rho} - \dot{\rho}) = [h, \rho^2 - \rho] \tag{2.36}$$

The solution of the TDHF equations will therefore trace a path on the energy surface of all the Slater determinants.

2.4.3 Conservation of Expectation Values of Symmetry Operators

For an arbitrary single-particle operator F with no time dependence,

$$F = \sum_{\alpha\beta} f_{\ell m} C_\ell^+ C_m \tag{2.37}$$

its expectation value in the state $|\Psi_{SD}\rangle$ is

$$i\hbar \frac{d}{dt}\langle F\rangle = i\hbar\, \mathrm{tr}(f\cdot\dot{\rho}) = \mathrm{tr}(f\cdot[h,\rho]) \tag{2.38}$$

Using Wicks theorem[50], we find that

$$\langle [F,H]\rangle = \mathrm{tr}(f\cdot[h,\rho]) \tag{2.39}$$

Hence

$$i\hbar \frac{d}{dt}\langle F\rangle = \langle [F,H]\rangle \tag{2.40}$$

We see that, on the average, all symmetries of the Hamiltonian are conserved. Examples are:

(i) conservation of the particle number

$$\frac{d}{dt}\langle N\rangle = \frac{d}{dt}(\mathrm{tr}\rho) = 0 \tag{2.41}$$

(ii) conservation of linear momentum

$$\frac{d}{dt}\langle \vec{P}\rangle = 0 \tag{2.42}$$

(iii) conservation of angular momentum

$$\frac{d}{dt}\langle \vec{J}\rangle = 0 \tag{2.43}$$

2.4.4 Conservation of Energy

Since ρ is always a Slater determinant, $\dot{\rho}$ only has ph matrix elements in the basis in which ρ is diagonal. Therefore we have

$$\frac{d}{dt}\langle H\rangle = \frac{d}{dt}E = \sum_{\alpha\beta}\left(\frac{\partial E}{\partial\rho_{\alpha\beta}}\dot{\rho}_{\alpha\beta} + \frac{\partial E}{\partial\rho_{\beta\alpha}}\dot{\rho}_{\beta\alpha}\right)$$

$$= \mathrm{tr}(h\cdot\dot{\rho}) = \frac{i}{\hbar}\,\mathrm{tr}(h\cdot[\rho,h]) = 0 \tag{2.44}$$

The energy is thus conserved with time. The motion has to take place on lines of constant energy on the multidimensional energy surface of Slater determinants.

2.4.5 Time Reversal Invariance

The one-body density $\rho(t)$ satisfying the TDHF equation (Eq. 2.13) is not time reversal invariant since the time reversal operator[51]

$$T = K_0\, e^{-i\sigma_y} \tag{2.45}$$

where K_0 is the complex conjugation, changes ρ ,

$$\rho_T(t) \equiv T\rho(t)T^{\dagger} \neq \rho(t) \tag{2.46}$$

because $\rho_T = \rho$ would require $\dot{\rho} = 0$. However, there is microscopic reversability, which means that $\rho_T(-t)$ also satisfies the TDHF equations.

2.4.6 Quasi-static Solutions

The TDHF equations can be related to the static Hartree-Fock equations by considering the class of single-particle wave functions in which the time dependence factors out:

$$\psi_j(\alpha,t) = e^{-i\epsilon_j t/\hbar}\,\psi_j(\alpha) \qquad (2.47)$$

where ϵ_j is the single-particle energy of the j-th particle. Substitution of this equation into Eq. 2.22 results in the static Hartree-Fock equations:

$$\sum_\beta h_{\alpha\beta}\,\psi_i(\beta) = \epsilon_j\,\psi_j(\alpha) \qquad (2.48)$$

With the effective interaction to be introduced in Chapter 3, such static solutions accuratly describe both the bulk and shell aspects of nuclear ground states.

In special cases we can readily find dynamical solutions to the TDHF equations from solutions of the static Hartree-Fock (HF) equations by a suitable transformation that breaks the time reversal symmetry. A gallilean transformation to a system moving with constant velocity $\vec{v}$ is such a transformation. It is realized by the operator G[51]

$$G(\vec{v},t) = \exp\left[-\frac{i}{\hbar}\vec{v}\cdot(mA\cdot\vec{R} - \vec{P}\cdot t)\right] \qquad (2.49)$$

where $\vec{R} = (1/A)\sum\vec{r}_i$ is the center of mass and $\vec{P} = \sum\vec{p}_i$ is the total momentum. The matrix in the single-particle space corresponding to this transformation is

$$g(\vec{v},t) = \exp\left[-\frac{i}{\hbar}\vec{v}\cdot(m\vec{r} - \vec{p}\,t)\right] \qquad (2.50)$$

which transforms the density

$$\rho(t) \longrightarrow \bar{\rho} = g\rho(t)g^{+} \tag{2.51}$$

$\bar{\rho}$ obeys the equation of motion

$$0 = i\hbar\dot{\bar{\rho}} = g[h,\rho]g^{+} - g[\vec{v}\cdot\hat{p},\rho]g^{+} = g[h(\rho)-\vec{v}\cdot\hat{p},\rho]\,g^{+} \tag{2.52}$$

Using Eq. 2.49 and the symmetry property

$$g\Gamma(\rho)g^{+} = \Gamma(\bar{\rho}) \tag{2.53}$$

which holds for gallilean-invariant interactions, the TDHF equations in the moving frame are

$$0 = i\hbar\dot{\bar{\rho}} = [h(\bar{\rho}),\bar{\rho}] \tag{2.54}$$

We thus see that $\bar{\rho}$ satisfies the static HF equation in the moving frame. $\bar{\rho}$ transforms into a nontrivial dynamic solution of the TDHF equations in the laboratory frame

$$\rho(t) = e^{(i/\hbar)m\vec{v}\cdot\vec{r}}\left(e^{-(i/\hbar)t\vec{v}\cdot\hat{p}}\,\bar{\rho}\,e^{(i/\hbar)t\vec{v}\cdot\hat{p}}\right)e^{-(i/\hbar)m\vec{v}\cdot\vec{r}} \tag{2.55}$$

The stationary solution $\bar{\rho}$ undergoes first a time-even translation of the coordinates by the amount $-\vec{v}t$ and then acquires a velocity by a time-odd transformation of the momenta. In applications of the TDHF theory to heavy-ion reactions, one often uses as initial condition a sum of two densities of the form of Eq. 2.49 with velocities $\vec{v}_1$ and $\vec{v}_2$ at a distance at which the overlap of the densities is considered negligible.

In the rotational case, we cannot transform the density ρ to a rotating system in which the motion can be described by a static HF solution. Nevertheless, a transformation to a frame rotating with the angular velocity $\vec{\omega}$,

$$\tilde{\rho} = e^{i\vec{\omega}\cdot\vec{j}t}\rho(t)\,e^{-i\vec{\omega}\cdot\vec{j}t} \tag{2.55}$$

leads to the stationary HF problem of the self-consistent cranking model:

$$[h(\tilde{\rho}) - \vec{\omega}\cdot\vec{j}\,,\,\tilde{\rho}\,] = 0 \tag{2.56}$$

We get a density $\tilde{\rho}$ with no time dependence but which contains time-odd components. In this sense $\tilde{\rho}$ is not a static density. Again,

$$\rho(t) = e^{-i\vec{\omega}\cdot\vec{j}t}\,\tilde{\rho}\,e^{i\vec{\omega}\cdot\vec{j}t} \tag{2.57}$$

is a nontrivial solution of the TDHF equations.

2.5 General Discussion of the TDHF Method

The TDHF method provides a consistent description of all types of collective motion, including fission. In the TDHF method, the nucleus determines for itself its own path on the multidimensional energy surface. It becomes unnecessary to choose beforehand the collective coordinates, or to subject the system to some physically unrealistic external fields.

Microscopically, the determinental wave function takes care of all the single-particle aspects and includes the full interplay between the collective and the single-particle motion. The TDHF equations have inherent one-body friction[52] produced by the interaction of the particles with the moving wall of a time-dependent mean-field.

In many instances, it is unclear how negligible the two-body correlations contained in the correlation function $g^{(2)}$ are. The approximation that the $g^{(2)}$ terms are negligible is based on the belief that the mean-free path of a nucleon, due to the Pauli exclusion principle, is of the order of the nuclear dimensions. This would no longer be the case if the single-particle energies are of the order of the Fermi energy. Modifications of the TDHF equations to include the effects of two-body collisions[39-44], if only in a phenomenological way, are unlikely to produce significant quantitative improvements of the present TDHF method. However, the TDHF method should still be able to describe a wide range of phenomena.

Although the TDHF method has many appealing advantages, the following should be noted:

(i) The TDHF method provides a fully microscopic description of the many-body system. Following each single-particle wave function as it changes with time requires a tremendous amount of numerical effort.

(ii) The theory has a classical deterministic behavior. Starting from an initial density $\rho(t)$, we follow it and its velocity $\dot{\rho}(t)$ through time on a multidimensional energy surface as if it were a classical trajectory. By restricting the wave function to a Slater determinant at all times, we end up with a set of coupled non-linear equations. We have therefore given up the superposition principle and we get solutions of a solition character, that is, density distributions which propagate without changing their shape (see e.g. Eq. 2.54).

Using Slater determinants as an approximation to the exact wave function puts us in the intrinsic system of the nucleus, thus requiring its center of mass coordinate and its momentum coordinate to be two simultaneously measurable quantities.

(iii) Conservation of energy prohibits the quantum-mechanical effect of tunneling through a potential barrier. For example, in the fission process, the fission barrier consists of a two-hump (and sometimes three-hump) potential barrier and any dynamical analysis by the TDHF method, from the initial stable nucleus through the barrier towards scission, is not possible. Negele et al.[18] in their examination of the spontaneous fission of ^{236}U, took their nucleus to be 1 MeV below and after the last saddle point energy. To introduce tunneling, we would need to either requantize or introduce linear superpositions of product states.

(iv) There exists fundamental questions in the physical interpretation of the results contained in the wave function $|\Psi_{SD}(t)\rangle$. Starting from a Slater determinant, the exact wave function $|\Psi(t)\rangle$ does not stay close to a Slater determinant in the course of time. It can be shown that the overlap $\langle\Psi(t)|\Psi_{SD}(t)\rangle$ can become very small when $|\Psi(t)\rangle$ is only slightly different from $|\Psi_{SD}(t)\rangle$. This does not mean however, that we cannot use $|\Psi_{SD}(t)\rangle$ for the evaluation of few-body operators. The stability of the TDHF determinant with respect to small perturbations can be examined in the Time Dependent Random-Phase approximation[33]. We shall use our results instead as an indirect measure of the stability of the TDHF method.

(v) In reaction theory, the initial value TDHF theory lacks asymptoticity. Due to the time dependence of the HF Hamiltonian

(Eq. 2.31) long after the collision, only a few "trajectory" characteristics remain constant once the fragments separate and they can unambiguously be obtained from the numerical TDHF studies of nuclear systems. This problem can be reinterpreted by using an analogy to the S-matrix form of the Schrodinger reaction theory[53,54]. In the TD-$\mathcal{S}$-HF reaction theory,

$$\bar{\mathcal{S}}_{fi} = (t_2 - t_1)^{-1} \int_{t_1}^{t_2} \langle \psi_f(\vec{r},t') \mid \psi_i(\vec{r},t') \rangle \, dt' \qquad (2.58)$$

describes the transition probability from an initial to a final self-consistent TDHF reaction channel.

(vi) The adiabatic limit of the TDHF equations, ATDHF, was proposed in 1978 by Baranger and Vénéroni[55,57]. A general density matrix satisfying

$$\rho^2 = \rho \qquad (2.59)$$

can be rewritten in the form

$$\rho = e^{(i/\hbar)\chi(t)} \rho_0(t) e^{-(i/\hbar)\chi(t)} \qquad (2.60)$$

where ρ_0 and χ are both Hermitian, time-even matrices, that is

$$\rho_T(t) \equiv T\rho(t)T^{\dagger} = e^{-(i/\hbar)\chi(t)} \rho_0(t) e^{(i/\hbar)\chi(t)} \qquad (2.61)$$

Again ρ_0 satisfies $\rho_0^2 = \rho_0$, $\mathrm{tr}\,\rho_0 = A$, which means that ρ_0 corresponds to an A-dimensional Slater determinant $|\Psi_{SD}(t)\rangle$. If χ is sufficiently small, implying all velocities are small, a systematic expansion can be developed in which approximate equations of motion for ρ_0 and χ

are determined from the TDHF equations. This formulation provides an elegant and general method for deriving a collective Hamiltonian which contains the usual simple potential energy term and the crucial mass parameters associated with each variable.

Chapter 3

THE ENERGY FUNCTIONAL

3.1 Introduction

The TDHF method consists of finding the solution of the many-body Schrodinger equation in a restricted Hilbert space, the ensemble of Slater determinants. This single-particle approximation of the dynamics of a nuclear system requires the definition of an effective Hamiltonian which will reproduce reasonably well the properties of the nucleus in such an unphysically restricted subspace.

There are essentially two groups of effective nucleon-nucleon interaction:

(i) In the first group the effective interaction is built up from a partial resummation of the scattering processes of two nucleons in nuclear matter[48,50,58-63]. The bare nucleon-nucleon interaction is then simply the Born term of this series. This type of interaction (also referred to as the G or K matrix) is termed effective because it acts in a restrictive subspace and consequently is modified to counter the effects of the neglected part of the Hilbert space. However, a phenomenological part must be added to the derived effective interaction in order to produce a satisfactory description of radii, binding energies, and single-particle energies of doubly-closed shell nuclei[64,65].

(ii) The second approach consists of assuming beforehand an analytical form for the effective nucleon-nucleon interaction. Although this direct parametrization is obviously less fundamental than the previous one, it has a certain number of advantages. First of all, the practical simplicity of the calculations involved give somewhat better physical insight, and simple relations connecting different nuclear properties can often be derived. Also, these phenomenological effective interactions are useful tools to extrapolate in a rather simple and reliable way to nuclei far from the stability line and to superheavy nuclei. An enormous number of different phenomenological effective interactions have been applied to problems in nuclear physics with tremendous success. However, most of them are constructed for a special purpose, as for example, those for Hartree-Fock calculations. Among these forces is the Skyrme interaction[28,35,49,66,67] which is the interaction to be used for this study.

In section 3.2 a general discussion of the Skyrme interaction is presented. Section 3.3 deals with the functional form of the energy to be used in the TDHF equations.

3.2 The Skyrme Interaction

It is well known that the nuclear force has a rather short range. The simplest ansatz therefore consists of using a zero range force whose radial dependence is described by a Dirac delta function δ. In 1956 Skyrme[66,67] proposed the following effective interaction[35]:

$$V = \sum_{i<j} v_{ij}^{(2)} + \sum_{i<j<k} v_{ijk}^{(3)} \tag{3.1}$$

with

$$\begin{aligned} v^{(2)}(\vec{r}_1,\vec{r}_2) = {} & t_0(1 + x_0 P^{\sigma})\,\delta(\vec{r}_1-\vec{r}_2) \\ & + \tfrac{1}{2} t_1 [\,\delta(\vec{r}_1-\vec{r}_2)\vec{k}^2 + \vec{k}'^2\delta(\vec{r}_1-\vec{r}_2)] \\ & + t_2 \vec{k}' \cdot \delta(\vec{r}_1-\vec{r}_2)\,\vec{k} \\ & + i V_{s.o.}(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}' \times \delta(\vec{r}_1-\vec{r}_2)\vec{k} \end{aligned} \tag{3.2}$$

and

$$v^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3) = t_3\,\delta(\vec{r}_1-\vec{r}_2)\,\delta(\vec{r}_2-\vec{r}_3) \tag{3.3}$$

In Eq. 3.2 P^{σ} is the spin exchange operator and $\vec{\sigma}$ represents the vector of the Pauli matrices, $\vec{k}$ is the operator

$$\frac{1}{2i}(\vec{\nabla}_1-\vec{\nabla}_2) \tag{3.4}$$

acting on the right and $\vec{k}'$ is the operator

$$-\frac{1}{2i}(\vec{\nabla}_1-\vec{\nabla}_2) \tag{3.5}$$

acting on the left. Here x_0, t_0, t_1, t_2, t_3 and the spin-orbit coupling strength $V_{s.o.}$, are the parameters of the interaction.

The momentum dependence of the two-body potential (Eq. 3.2) simulates a finite non-vanishing range[68,69]. This can readily be seen[36] by comparing the matrix elements of Eq. 3.2 in momentum space

$$\langle\vec{k}\,|\,v_{12}^{(2)}\,|\,\vec{k}'\rangle = t_0(1+x_0P^{\sigma}) + \frac{1}{2}t_1(\vec{k}^2+\vec{k}'^2) + t_2\,\vec{k}'\cdot\vec{k} + iV_{s.o.}(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}'\times\vec{k} \tag{3.6}$$

with a Taylor series expansion of a Gaussian central force with exchange terms,

$$V = e^{-(r_{12}/\mu)^2}(W+BP^{\sigma}-HP^{\tau}-MP^{\sigma}P^{\tau}) \tag{3.7}$$

in momentum space,

$$\langle \vec{K} | V | \vec{K}' \rangle = (\mu\sqrt{\pi})^3 [W + M + (B+H) P^\sigma][1 - \tfrac{1}{4}(\vec{K}^2 - \vec{K}'^2)\mu^2] + \tfrac{1}{2}(\mu\sqrt{\pi})^3 [W - M + (B-H)P^\sigma]\mu^2 \, \vec{K}\cdot\vec{K}' \tag{3.8}$$

Eq. 3.8 is identical to Eq. 3.6 except for the last term. One can also show[70] that this last term can be generated by a two-body spin-orbit force $V_{so}(r_{12})\vec{L}\cdot\vec{S}$, where in the short-range limit

$$V_{S.O.} = -\tfrac{2}{3}\pi \int_0^\infty V_{LS}(r)\, r^4 \, dr \tag{3.9}$$

By considering the matrix elements of expression 3.2 in a state of relative motion,

$$\Psi(\vec{r}) = R(r)\, Y_{\ell m}(\Omega) \tag{3.10}$$

one can see[66,67] that the first two terms correspond to S-wave interactions since the matrix elements are proportional to $|\Psi(0)|^2$ and $\Psi(0)\nabla^2\Psi(0)$, respectively; whereas the last two terms correspond to P-wave interactions since the matrix elements are proportional to $|\vec{\nabla}\Psi(0)|^2$.

The Skyrme effective interaction depends on the density $\rho(\vec{r})$. Such a density dependence is necessary[29,48,71] and can be understood by considering the following expression for the G-matrix (Bethe-Goldstone equation[61,72])

$$G^E_{ab,cd} = \bar{v}_{ab,cd} + \frac{1}{2}\sum_{m,n>\epsilon_F} \bar{v}_{ab,mn} \frac{1}{E - \epsilon_m - \epsilon_n + i\eta} G^E_{mn,cd} \tag{3.11}$$

where ab,...,mn are shell-model indices and ϵ_F is the Fermi energy. The range of the summation depends on the Fermi energy which is itself a function of the density, producing some density dependence in the effective nuclear interaction. For spin saturated even-even nuclei, the three-body term given in Eq. 3.3 is equivalent[36] to a density dependent two-body interaction of the form of

$$v_\rho(\vec{r}_1,\vec{r}_2) = \frac{1}{6}t_3(1+P^\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho\left(\tfrac{1}{2}(\vec{r}_1+\vec{r}_2)\right) \qquad (3.12)$$

This interpretation is preferable to the view that the Skyrme contains a three-body interaction, since three-body interactions in nuclei are relatively weak. For systems without spin saturation, the three-body term given in Eq. 3.3 favors parallel spin alignment. This contradicts the observed spin saturation and the pairing properties in nuclei. This difficulty is overcome by using either a density dependent two-body interaction[73] of the form of Eq. 3.12 or a nonlocality in the three-body term[74].

There are three main reasons for using this force:

(i) Vautherin and Brink[36] performed spherical static HF calculations and were able to reproduce the binding energies and radii of doubly-closed shell nuclei across the periodic table with reasonable sets of parameters. Over the last decade or so, numerous calculations (see sec. 2.1) have had success in the study of nuclear systems.

(ii) Negele and Vautherin[37] showed that the Skyrme effective interaction is connected with the more fundamental G matrix of nuclear matter.

(iii) The mathematical form of the force is extremely simple. The δ-functions reduce the TDHF equations to a set of nonlinear differential equations which simplifies the calculations enormously.

3.3 The Energy Functional

The calculations to be presented use a modified Skyrme form for the nuclear interaction together with the Coulomb interaction[18,28,35,36,49]. The total energy for the system, $\mathcal{H}$ is thus

$$\mathcal{H} = \mathcal{H}_n + \mathcal{H}_c \tag{3.13}$$

where $\mathcal{H}_n$ is the nuclear energy and $\mathcal{H}_c$ is the Coulomb energy.

3.3.1 The Nuclear Energy

The nuclear energy is given by

$$\begin{aligned}\mathcal{H}_n &= \langle \Psi_{S.D} | t + v | \Psi_{S.D} \rangle \\ &= \sum_i \langle i | \frac{p^2}{2m} | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | \bar{v}_{12}^{(2)} | ij \rangle + \frac{1}{6} \sum_{ijk} \langle ijk | \bar{v}_{ijk}^{(3)} | ijk \rangle \\ &= \int H_n(\vec{r})\, d\vec{r}\end{aligned} \tag{3.14}$$

where $\bar{v}$ denotes the antisymmetrized matrix element. For the Skyrme interaction the energy density $H_n(\vec{r})$ is an algebraic function of the nucleon densities (ρ_n and ρ_p), the kinetic energy densities (τ_n and τ_p), and the current densities ($\vec{j}_n, \vec{j}_p$). For an even-even nucleus, we assume that we have a spin-saturated system so that each spatial orbital is occupied by a spin $\frac{1}{2}$ and a spin $-\frac{1}{2}$ nucleon. Neglecting the presumably small effects due to the spin-orbit force, the Skyrme form of the nuclear density[29,35,36] is

$$
\begin{aligned}
H_n(\vec{r}) = {} & \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left[(1+\frac{1}{2}x_0)\rho^2 - (x_0+\frac{1}{2})(\rho_n^2+\rho_p^2)\right] \\
& + \frac{1}{4}(t_1+t_2)(\rho\tau - j^2) + \frac{1}{8}(t_2-t_1)(\rho_n\tau_n + \rho_p\tau_p - j_n^2 - j_p^2) \\
& + \frac{1}{16}(t_2-3t_1)\rho\nabla^2\rho + \frac{1}{32}(t_2+3t_1)(\rho_n\nabla^2\rho_n + \rho_p\nabla^2\rho_p) \\
& + \frac{1}{4}t_3\rho_n\rho_p\rho
\end{aligned}
\tag{3.15}
$$

The particle, kinetic energy, and current densities for each isospin species q (p for protons, n for neutrons) are defined as

$$\rho_q(\vec{r}) = \sum_{\alpha\in q} n_\alpha |\psi_\alpha(\vec{r})|^2 \tag{3.16a}$$

$$\tau_q(\vec{r}) = \sum_{\alpha\in q} n_\alpha |\vec{\nabla}\psi_\alpha(\vec{r})|^2 \tag{3.16b}$$

$$j_q(\vec{r}) = \sum_{\alpha\in q} n_\alpha \, \mathrm{Im}\left[\psi_\alpha^*(\vec{r})\vec{\nabla}\psi_\alpha(\vec{r})\right] \tag{3.16c}$$

where the sums are over all the single-particle orbitals; n_α is the occupation number of the α-th orbital and has values 2 or 0 depending on whether the orbital is populated by a pair of nucleons or not. The densities in Eq. 3.15 without isospin subscripts refer to the total density ($\rho = \rho_n + \rho_p$, $\tau = \tau_n + \tau_p$, $j = j_n + j_p$). In time-dependent calculations, all of the functions in Eq. 3.17 depend on time t as well as on the spatial coordinates $\vec{r}$.

The parameters t_0, t_1, t_2, t_3 and x_0 appearing in Eq. 3.15 are the usual constants of the Skyrme force[29,36]. Vautherin and Brink determined them in the following way[36]. First of all, the parameters were adjusted to fit the binding energy and density of nuclear matter, as well as the binding energies of helium-4, oxygen-16, and calcium-40.

This procedure determines the four parameters t_0, t_1, t_2, t_3. The parameter x_0, which determines the symmetry effects, was adjusted to give a value of 30 MeV for the symmetry-energy coefficient in nuclear matter. Then static HF calculations were carried out for doubly-closed shell nuclei. The parameters were then corrected to obtain a better fit for oxygen-16 and lead-208. Using this procedure Vautherin and Brink found several sets of parameters giving a good description of closed-shell nuclei in HF calculations. Our choice of parameters are those for the Skyrme-II interaction and are given in Table I. With this force[28,36], nuclear matter saturates at a density $\rho = 0.15\ \mathrm{fm}^{-3}$ corresponding to a Fermi momentum of 1.30 fm and a binding energy per nucleon of 16.0 MeV, an incompressibility coefficient of 340 MeV, and a symmetry energy coefficient of 34.1 MeV. The binding energies and radii calculated with this force for nuclei over a wide range of the periodic table are in good agreement with experiment[36].

In order to improve the stability of the numerical calculations, it was found[2,18,28] to be convenient to replace the surface energy terms in Eq. 3.15 of the form $\rho\nabla^2\rho$ by the following sum of direct Yukawa interactions[49]

$$H_Y(\vec{r}) = \int d\vec{r}\,' \frac{e^{-|\vec{r}-\vec{r}\,'|/a}}{|\vec{r}-\vec{r}\,'|/a} \Big[\frac{V_\ell}{2}\big(\rho_n(\vec{r})\rho_n(\vec{r}\,') + \rho_p(\vec{r})\rho_p(\vec{r}\,') + \frac{V_u}{2}\big(\rho_n(\vec{r})\rho_p(\vec{r}\,') + \rho_p(\vec{r})\rho(\vec{r}\,')\big)\Big]$$

where V_ℓ and V_u are the strengths of the interactions between "like" and "unlike" nucleons. Comparison of Eq. 3.15 with a Taylor series expansion of Eq. 3.18 gives the following relations between the parameters of the Skyrme force and V_ℓ and V_μ :

$$2\pi V_\mu a^5 = \frac{1}{16}(t_2 - 3t_1) \tag{3.18a}$$

$$2\pi(V_\ell - V_\mu) = \frac{1}{32}(t_2 + 3t_1) \tag{3.18b}$$

The value of a is chosen to approximate the range of the G-matrix in nuclear matter[2]. Defining the new parameters $\tilde{t}_0$ and $\tilde{x}_0$ by

$$\frac{1}{2}\tilde{t}_0\left(1 + \frac{\tilde{x}_0}{2}\right) = \frac{1}{2}t_0\left(1 + \frac{x_0}{2}\right) - 2\pi a^3 V_\mu \tag{3.19a}$$

$$\frac{1}{2}\tilde{t}_0\left(\frac{1}{2} + \tilde{x}_0\right) = \frac{1}{2}t_0\left(\frac{1}{2} + x_0\right) + 2\pi a^3 (V_\ell - V_\mu) \tag{3.19b}$$

the nuclear energy density becomes

$$\begin{aligned} H_n(\vec{r}) = {} & \frac{\hbar^2}{2m}\tau + \frac{1}{2}\tilde{t}_0\left[\left(1 + \frac{\tilde{x}_0}{2}\right)\rho^2 - \left(\tilde{x}_0 + \frac{1}{2}\right)(\rho_n^2 + \rho_p^2)\right] \\ & + \frac{1}{4}(t_1 + t_2)(\rho\tau - j^2) + \frac{1}{8}(t_2 - t_1)(\rho_n\tau_n + \rho_p\tau_p - j_n^2 - j_p^2) \\ & + \frac{1}{4}t_3\rho_n\rho_p\rho + H_\gamma(\vec{r}) \end{aligned} \tag{3.20}$$

The parameters are listed in Table I.

TABLE I. The parameters t_0(Mev fm^3), x_0, $\tilde{t}_0$ (MeV fm^3), $\tilde{x}_0$, t_1(MeV fm^5), t_2(MeV fm^5), t_3(MeV fm^6), V_ℓ (MeV), V_μ(MeV), and a (fm) of the Skyrme II and modified Skyrme II interactions (Refs. 28,36,49).

t_0	x_0	$\tilde{t}_0$	$\tilde{x}_0$	t_1	t_2	t_3	V_ℓ	V_μ	a
-1169.9	0.34	-104.49	4.01	585.6	-27.1	9331.0	-444.85	-863.53	0.45979

3.3.2 The Coulomb Energy

The Coulomb energy density can be seperated into two parts:

$$H_c(\vec{r}) = H_c^{(dir)}(\vec{r}) + H_c^{(ex)}(\vec{r}) \tag{3.21}$$

The direct term is

$$H_c^{(dir)}(\vec{r}) = \frac{1}{2} e^2 \int d\vec{r}' \rho_p(\vec{r}) \frac{1}{|\vec{r}-\vec{r}'|} \rho_p(\vec{r}') \tag{3.22}$$

For the exchange term, we assume that the ratio of the direct Coulomb energy to the exchange Coulomb energy is the same as in nuclear matter. This is called the Slater approximation[75]. Combining this approximation with a local density approximation[37,76], we get the following form for the exchange Coulomb energy density:

$$H_c^{(ex)}(\vec{r}) = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1\text{[illegible]}} e^2 \left[\rho_p(\vec{r})\right]^{4/3} \tag{3.23}$$

This approximation to the Coulomb energy density was found to be in qualitative agreement with exact calculations[77]. TDHF studies of light-ion systems have also shown that the inclusion of $H_c^{(ex)}$ has negligible effects on experimental observables[14]. Eq. 3.23 should therefore be sufficient for the present calculations.

3.3.3 Specialization to Axial Symmetry

Assuming that the nuclear system is axially symmetric, we express the energy density functional in cylindrical coordinates $\vec{r} = (r,z,\phi)$[6,49]. The single-particle wave functions can then be written in the form

$$\psi_\alpha(\vec{r}) = \psi_\alpha(r,z)\, e^{i\mu_\alpha \phi} \tag{3.24}$$

where μ_α is the azimuthal quantum number of the orbital α.

The energy density functional (Eqs. 3.20, 3.22, 3.23) can be written as

$$H(\vec{r}) = H_0(\vec{r}) + H_H(\vec{r}) + H_V(\vec{r}) \tag{3.25}$$

where $H_0(\vec{r})$ contains the derivative-independent parts of $H(\vec{r})$, H_H contains the terms in $H(\vec{r})$ arising from the z derivatives, and H_V contains the terms in $H(\vec{r})$ arising from the r and ϕ derivatives. In detail[49],

$$H_0(\vec{r}) = \frac{1}{2}\tilde{t}_0\left[\left(1 + \frac{\tilde{x}_0}{2}\right)\rho^2 - \left(\frac{1}{2} + \tilde{x}_0\right)(\rho_n^2 + \rho_p^2)\right] + \frac{1}{4}t_3\rho_n\rho_p\rho + H_Y(\vec{r}) + H_c(\vec{r}) \tag{3.26}$$

$$H_H(\vec{r}) = \frac{\hbar^2}{2m}\tau_z + \frac{1}{4}(t_1 + t_2)(\rho\tau_z - j_z^2) + \frac{1}{8}(t_2 - t_1)(\rho_n\tau_{zn} + \rho_p\tau_{zp} - j_{zn}^2 - j_{zp}^2) \tag{3.27}$$

$$H_V(\vec{r}) = \frac{\hbar^2}{2m}(\tau_r + s) + \frac{1}{4}(t_1 + t_2)\left[\rho(\tau_r + s) - j_r^2\right] + \frac{1}{8}(t_2 - t_1)\left[\rho_n(\tau_{rn} + S_n) + \rho_p(\tau_{rp} + S_p) - j_{rn}^2 - j_{rp}^2\right] \tag{3.28}$$

where the following "components" of the various densities are defined as

$$\tau_{zq} = \sum_{\alpha\in q} n_\alpha \left|\frac{\partial\psi_\alpha}{\partial z}\right|^2 \tag{3.29a}$$

$$\tau_{rq} = \sum_{\alpha\in q} n_\alpha \left|\frac{\partial\psi_\alpha}{\partial r}\right|^2 \tag{3.29b}$$

$$S_q = \sum_{\alpha\in q} n_\alpha \frac{\mu_\alpha^2}{r^2}\left|\psi_\alpha\right|^2 \tag{3.29c}$$

$$j_{zq} = \sum_{\alpha\in q} n_\alpha \, \mathrm{Im}\left(\psi_\alpha^* \frac{\partial\psi_\alpha}{\partial z}\right) \tag{3.29d}$$

$$j_{rq} = \sum_{\alpha\in q} n_\alpha \, \mathrm{Im}\left(\psi_\alpha^* \frac{\partial\psi_\alpha}{\partial r}\right) \tag{3.29e}$$

Since we assumed equal occupation of pairs of orbitals having equal and opposite azimuthal quantum numbers, the term

$$j_{\phi q} = \sum_{\alpha\in q} \eta_\alpha \mu_\alpha \, \mathrm{Im}(i\, \psi_\alpha^* \psi_\alpha) \tag{3.30}$$

vanishes.

Chapter 4

CALCULATION DETAILS

4.1 Introduction

The TDHF equations are a set of non-linear coupled equations. An exact solution is possible only in very special cases[78]. In the present study no exact solution of the TDHF equations is possible and numerical methods must be used. We solve the TDHF equations by finite difference methods on a cylindrical mesh[6,28,49]. The most useful discrete representation of the TDHF Hamiltonian is obtained by the variation of a discrete approximation to the energy functional with respect to the values of the single-particle wave functions at the mesh points.

In section 4.2 the spatial discretization is performed while the time discretization is done in section 4.3. The Static Hartree-Fock problem is discussed in section 4.4. Section 4.5 deals with the calculation of the total and single-particle energies. Other calculational details are presented in section 4.6.

4.2 Spatial Discretization

We take the nucleus to be axially symmetric along the z-axis. The mesh along the z-direction is defined by

$$z_j = (j-1)\Delta z \qquad , \; j = 1,2,\ldots, N_z \tag{4.1}$$

In specifying the mesh points along the radial direction, it is advantageous to choose the points at half-integral multiples of the mesh spacing:

$$r_i = (i-\tfrac{1}{2})\Delta r \qquad , i = 1,2,\ldots, N_R \tag{4.2}$$

This is done in order to avoid the singularity at $r=0$.

Each single-particle wave function is represented by its values on the mesh points,

$$\psi_\alpha(i,j) \equiv \psi_\alpha(r_i, z_j) \tag{4.3}$$

The single-particle wave functions are normalized with

$$\sum_{i=1}^{N_R} \sum_{j=1}^{N_z} |\psi_\alpha(i,j)|^2 \Delta V_i = 1 \tag{4.4}$$

where the volume element is

$$\Delta V_i = 2\pi (i-\tfrac{1}{2})(\Delta r)^2 \Delta z \tag{4.5}$$

To avoid any mass loss from our discretized space, we need to impose the following boundary conditions

$$\begin{aligned} &\psi_\alpha(N_R, j) = 0 && , j = 1,2,\ldots,N_z \\ &\psi_\alpha(i,1) = \psi_\alpha(i,N_z) = 0 && , i = 1,2,\ldots,N_R \end{aligned} \tag{4.6}$$

4.2.1. Spatial Discretization of the Energy Functional

To discretize the energy functional given by equation 3.26, it is useful to define[49]

$$g_\alpha(i,j) = (i-\tfrac{1}{2})^{1/2} \psi_\alpha(i,j) \tag{4.7}$$

The normalization condition then takes the simple form.

$$2\pi(\Delta r)^2 \Delta z \sum_{i=1}^{N_R} \sum_{j=1}^{N_Z} |g_\alpha(i,j)|^2 = 1 \tag{4.8}$$

and the boundary conditions are

$$\begin{aligned} g_\alpha(N_R, j) &= 0 \qquad\qquad j = 1,2,\ldots,N_Z \\ g_\alpha(i,1) = g_\alpha(i,N_Z) &= 0 , \quad i = 1,2,\ldots,N_R \end{aligned} \tag{4.9}$$

The discrete approximations to the densities (Eqs. 3.29) are[49]

$$\rho_q(i,j) = \frac{1}{(i-\frac{1}{2})} \sum_{\alpha\in q} n_\alpha |g_\alpha(i,j)|^2 \tag{4.10a}$$

$$\rho_{zq}(i,j+\tfrac{1}{2}) = \tfrac{1}{2}\left[\rho_q(i,j) + \rho_q(i,j+1)\right] \tag{4.10b}$$

$$\rho_{rq}(i+\tfrac{1}{2},j) = \tfrac{1}{2}\left[\rho_q(i,j) + \rho_q(i+1,j)\right] \tag{4.10c}$$

$$\tau_{zq}(i,j+\tfrac{1}{2}) = \frac{1}{(i-\frac{1}{2})(\Delta z)^2} \sum_{\alpha\in q} n_\alpha |g_\alpha(i,j) - g_\alpha(i,j+1)|^2 \tag{4.10d}$$

$$\tau_{rq}(i+\tfrac{1}{2},j) = \frac{1}{(i-\frac{1}{2})(\Delta r)^2} \sum_{\alpha\in q} n_\alpha i \left| \frac{g_\alpha(i,j)}{\sqrt{i-\frac{1}{2}}} - \frac{g_\alpha(i+1,j)}{\sqrt{i+\frac{1}{2}}} \right|^2 \tag{4.10e}$$

$$S_q(i,j) = \frac{1}{(i-\frac{1}{2})^3(\Delta r)^2} \sum_{\alpha\in q} n_\alpha \mu_\alpha^2 |g_\alpha(i,j)|^2 \tag{4.10f}$$

$$j_{zq}(i,j+\tfrac{1}{2}) = \frac{1}{(i-\frac{1}{2})(\Delta z)} \sum_{\alpha\in q} n_\alpha \, \mathrm{Im}\left[g_\alpha^*(i,j)\, g_\alpha(i,j+1)\right] \tag{4.10g}$$

$$j_{rq}(i+\tfrac{1}{2},j) = \frac{1}{(i-\frac{1}{2})(\Delta r)} \sum_{\alpha\in q} n_\alpha \left(\frac{i}{i+\frac{1}{2}}\right)^{1/2} \mathrm{Im}\left[g_\alpha^*(i,j)\, g_\alpha(i+1,j)\right] \tag{4.10h}$$

Taking care to properly center the difference formulas, Eqs. 3.27 may be written as[49]

$$
\begin{aligned}
H_0(i,j) = {} & \frac{1}{2}\tilde{t}_0\left[\left(1+\frac{\tilde{x}_0}{2}\right)\rho^2(i,j) - \left(\frac{1}{2}+\tilde{x}_0\right)\left(\rho_p^2(i,j)+\rho_n^2(i,j)\right)\right] \\
& + \frac{t_3}{4}\left[\rho(i,j)\,\rho_n(i,j)\,\rho_p(i,j)\right] \\
& - \frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} e^2\left[\rho_p(i,j)\right]^{4/3} + H_Y(i,j) + H_C^{(\mathrm{Dir})}(i,j)
\end{aligned} \tag{4.11a}
$$

$$
\begin{aligned}
H_H(i,j) = {} & \frac{\hbar^2}{2m}\tau_z(i,j+\tfrac{1}{2}) + \frac{t_1+t_2}{4}\left[\rho_z(i,j+\tfrac{1}{2})\tau_z(i,j+\tfrac{1}{2}) - j_z^2(i,j+\tfrac{1}{2})\right] \\
& + \frac{t_2-t_1}{8}\sum_q\left[\rho_{zq}(i,j+\tfrac{1}{2})\tau_{zq}(i,j+\tfrac{1}{2}) - j_{zq}^2(i,j+\tfrac{1}{2})\right]
\end{aligned} \tag{4.11b}
$$

$$
\begin{aligned}
H_V(i,j) = {} & \frac{\hbar^2}{2m}\left[\tau_r(i+\tfrac{1}{2},j) + s(i,j)\right] \\
& + \frac{t_1+t_2}{4}\left[\rho_r(i+\tfrac{1}{2},j)\tau_r(i+\tfrac{1}{2},j) + \rho(i,j)s(i,j) - j_r^2(i+\tfrac{1}{2},j)\right] \\
& + \frac{t_2-t_1}{8}\sum_q\left[\rho_{rq}(i+\tfrac{1}{2},j)\tau_{rq}(i+\tfrac{1}{2},j) + \rho_q(i,j)s_q(i,j) - j_{rq}^2(i+\tfrac{1}{2},j)\right]
\end{aligned} \tag{4.11c}
$$

The discrete approximations to the finite-range Yukawa and direct Coulomb energies are presented in section 4.2.3.

4.2.2 Spatial Discretization of the TDHF Equations

The discretized TDHF equations used are found variationally by discretizing the action $\mathcal{S}$ (Eq. 2.30):

$$
\begin{aligned}
\mathcal{S} = \int dt\,\Big\{\sum_{ij}\Delta V_i\Big[\sum_\alpha \psi_\alpha^*(i,j)\, i\hbar\,\frac{\partial\psi_\alpha(i,j)}{\partial t} - H_0(i,j) \\
- H_H(i,j) - H_V(i,j)\Big]\Big\}
\end{aligned} \tag{4.12}
$$

The variation of Eq. 4.12 with respect to $g_\alpha^*(i,j)$ results in TDHF equations of the form

$$i\hbar \frac{\partial g_\alpha(i,j)}{\partial t} = (\tilde{H} g_\alpha)(i,j) + (\tilde{V} g_\alpha)(i,j) \tag{4.13}$$

The "horizontal" Hamiltonian operator $\tilde{H}$ is defined by[49]

$$\begin{aligned}(\tilde{H} g_\alpha)(i,j) = {} & B_q^{(+)}(i,j)\, g_\alpha(i,j+1) \\ & + B_q^{(+)*}(i,j-1)\, g_\alpha(i,j-1) \\ & + \left[B_q^{(0)}(i,j) + \tfrac{1}{2} h_{oq}(i,j)\right] g_\alpha(i,j)\end{aligned} \tag{4.14}$$

and the "vertical" Hamiltonian operator $\tilde{V}$ is defined by

$$\begin{aligned}(\tilde{V} g_\alpha)(i,j) = {} & A_q^{(+)}(i,j)\, g_\alpha(i+1,j) \\ & + A_q^{(+)*}(i\text{[illegible]},j)\, g_\alpha(i-1,j) \\ & + \left[A_{\mu q}^{(0)}(i,j) + \tfrac{1}{2} h_{oq}(i,j)\right] g_\alpha(i,j)\end{aligned} \tag{4.15}$$

The quantity $h_{oq}(i,j)$ results from the variation of $H_o(i,j)$ and is given by[49]

$$\begin{aligned}h_{oq}(i,j) = {} & \tilde{t}_o\left[\left(1 + \frac{\tilde{x}_o}{2}\right)\rho(i,j) - \left(\tfrac{1}{2} + \tilde{x}_o\right)\rho_q(i,j)\right] \\ & + \frac{t_3}{2}\rho_n(i,j)\rho_p(i,j) + V_u\, \mathcal{U}_Y(i,j) \\ & + (V_\ell - V_u)\, \mathcal{U}_{Yq}(i,j) \\ & + \delta_{qp}\left[\mathcal{U}_c(i,j) - \left(\frac{3}{\pi}\right)^{1/3} e^2 \rho_p^{1/3}(i,j)\right]\end{aligned} \tag{4.16}$$

where $U_{yq}(i,j)$ and $U_c(i,j)$ denote the discrete approximations to the Yukawa and direct Coulomb potentials,

$$U_{yq}(\vec{r}) = \int d\vec{r}\,' \; \frac{e^{-|\vec{r}-\vec{r}\,'|/a}}{|\vec{r}-\vec{r}\,'|/a} \; \rho_q(\vec{r}\,') \tag{4.17a}$$

$$U_c(\vec{r}) = e^2 \int d\vec{r}\,' \; \frac{1}{|\vec{r}-\vec{r}\,'|} \; \rho_p(\vec{r}\,') \tag{4.17b}$$

The evaluation of Eqs. 4.17 is discussed in section 4.2.3.

The quantities B_q come from the variation of $H_H(i,j)$ [49]:

$$\begin{aligned} B_q^{(0)}(i,j) = \frac{\hbar^2}{m(\Delta z)^2} &+ \frac{t_1+t_2}{4}\Big\{ \frac{\rho_z(i,j+\frac{1}{2}) + \rho_z(i,j-\frac{1}{2})}{(\Delta z)^2} \\ &\qquad + \tfrac{1}{2}\big[\tau_z(i,j+\tfrac{1}{2}) + \tau_z(i,j-\tfrac{1}{2})\big]\Big\} \\ &+ \frac{t_2-t_1}{8}\Big\{ \frac{\rho_{zq}(i,j+\frac{1}{2}) + \rho_{zq}(i,j-\frac{1}{2})}{(\Delta z)^2} \\ &\qquad + \tfrac{1}{2}\big[\tau_{zq}(i,j+\tfrac{1}{2}) + \tau_{zq}(i,j-\tfrac{1}{2})\big]\Big\} \end{aligned} \tag{4.18}$$

$$\begin{aligned} B_q^{(1)}(i,j) = \frac{-\hbar^2}{2m(\Delta z)^2} &- \left[\left(\frac{t_1+t_2}{4(\Delta z)^2}\right)\rho_z(i,j+\tfrac{1}{2}) + \left(\frac{t_2-t_1}{8(\Delta z)^2}\right)\rho_{zq}(i,j+\tfrac{1}{2})\right] \\ &+ \sqrt{-1}\left[\left(\frac{t_1+t_2}{4(\Delta z)}\right)j_z(i,j+\tfrac{1}{2}) + \left(\frac{t_2-t_1}{8(\Delta z)}\right)j_{zq}(i,j+\tfrac{1}{2})\right] \end{aligned} \tag{4.19}$$

Similarly, the A_q are obtained from the variation of $H_V(i,j)$ [49]:

$$A_{\mu q}^{(0)}(i,j) = C_{\mu q}(i,j) + D_q(i,j) \tag{4.20}$$

$$C_{\mu q}(i,j) = \frac{\mu^2}{r_i^2}\left[\frac{\hbar^2}{2m} + \left(\frac{t_1+t_2}{4}\right)\rho(i,j) + \left(\frac{t_2-t_1}{8}\right)\rho_q(i,j)\right] \tag{4.21}$$

$$\begin{aligned} D_q(i,j) = {} & \frac{\hbar^2}{m(\Delta r)^2} + \left(\frac{t_1+t_2}{4}\right)s(i,j) + \left(\frac{t_2-t_1}{8}\right)s_q(i,j) \\ & + \frac{t_1+t_2}{4(i-\frac{1}{2})}\left\{\frac{i\rho_r(i+\frac{1}{2},j) + (i-1)\rho_r(i-\frac{1}{2},j)}{(\Delta r)^2}\right. \\ & \left. + \frac{1}{2}\left[(i-\tfrac{1}{2})\tau_r(i+\tfrac{1}{2},j) + (i-\tfrac{3}{2})\tau_r(i-\tfrac{1}{2},j)\right]\right\} \\ & + \frac{t_2-t_1}{8(i-\frac{1}{2})}\left\{\frac{i\rho_{rq}(i+\frac{1}{2},j) + (i-1)\rho_{rq}(i-\frac{1}{2},j)}{(\Delta r)^2}\right. \\ & \left. + \frac{1}{2}\left[(i-\tfrac{1}{2})\tau_{rq}(i+\tfrac{1}{2},j) + (i-\tfrac{3}{2})\tau_{rq}(i-\tfrac{1}{2},j)\right]\right\} \end{aligned} \tag{4.22}$$

$$\begin{aligned} A_q^{(+)}(i,j) = {} & \frac{-i}{(i^2-\frac{1}{4})^{1/2}(\Delta r)^2}\left[\frac{\hbar^2}{2m} + \left(\frac{t_1+t_2}{4}\right)\rho_r(\text{[illegible]}\tfrac{1}{2},j) + \left(\frac{t_2-t_1}{8}\right)\rho_{rq}(i+\tfrac{1}{2},j)\right] \\ & + \frac{\sqrt{-1}}{\Delta r}\left(\frac{i}{i-\frac{1}{2}}\right)^{1/2}\left[\left(\frac{t_1+t_2}{4}\right)j_r(i+\tfrac{1}{2},j) + \left(\frac{t_2-t_1}{8}\right)j_{rq}(i+\tfrac{1}{2},j)\right] \end{aligned} \tag{4.23}$$

The operators $\tilde{H}$ and $\tilde{V}$ are seen to be Hermitian operators and hence give rise to a unitary evolution. For each row i, the horizontal Hamiltonian operator $\tilde{H}$ can be represented by a tridiagonal matrix H acting towards the left:

$${}^{(i,q)}H_{\ell j} = \begin{cases} B_q^{(+)}\text{[illegible]}-1) & \ell = j-1 \\ B_q^{\text{[illegible]}}(i,j) + \frac{1}{2}h_{oq}(i,j) & \ell = j \\ B_q^{(+)}(i,j) & \ell = j+1 \\ 0 & \text{elsewhere} \end{cases} \tag{4.24}$$

Similarly, for each column j, the vertical Hamiltonian operator $\tilde{V}$ can be represented by a tridiagonal matrix V acting towards the right:

$$ {}^{(j,q)}V_{i\ell}^{(\mu)} = \begin{cases} A_q^{(+)*}(i-1,j) & \ell = i-1 \\ A_{\mu q}^{(0)}(i,j) + \frac{1}{2} h_{0q}(i,j) & \ell = i \\ A_q^{(+)}(i,j) & \ell = i+1 \\ 0 & \text{elsewhere} \end{cases} \qquad (4.25)$$

4.2.3 Evaluation of the Yukawa and Coulomb Potentials

In order to determine directly the Yukawa potential

$$U_{Yq}(\vec{r}) = V_0 \int d\vec{r}\,' \; \frac{e^{-|\vec{r}-\vec{r}\,'|/a}}{|\vec{r}-\vec{r}\,'|/a} \; \rho_q(\vec{r}\,') \qquad (4.26)$$

and the Coulomb potential

$$U_c(\vec{r}) = e^2 \int d\vec{r}\,' \; \frac{1}{|\vec{r}-\vec{r}\,'|} \; \rho_p(\vec{r}\,') \qquad (4.27)$$

by numerical integration, $N_R \times N_z$ folding would be required at each time step. This is very time consuming if N_R and N_z are large. We shall therefore consider the evaluation of the Yukawa and Coulomb potentials according to the method outlined in reference 6. The constant V_0 appearing in Eq. 4.26 will be set to 1 to get equation 4.17a. First we note that the Yukawa potential satisfies the Helmholtz equation

$$-\nabla^2 U_{Yq}(\vec{r}) + \frac{1}{a^2} U_{Yq}(\vec{r}) = 4\pi a \rho_q(\vec{r}) \qquad (4.28)$$

and the Coulomb potential satisfies the Poisson equation

$$-\nabla^2 U_c(\vec{r}) = 4\pi e^2 \rho_p(\vec{r}) \tag{4.29}$$

Eq. 4.29 can be seen to be a limiting case of Eq. 4.28 where

$$a \rightarrow \infty, \quad V_0 \rightarrow 0, \quad V_0 a \rightarrow e^2 \tag{4.30}$$

therefore we will only need to consider Eq. 4.28. Defining

$$\phi(i,j) = \sqrt{r_i}\, U_{Yq}(r_i, z_j) \tag{4.31a}$$

$$S(i,j) = \sqrt{r_i}\, 4\pi a V_0\, \rho_q(r_i, z_j) \tag{4.31b}$$

Eq. 4.28 is approximated on the mesh by

$$[(\tilde{H} + \tilde{V})\phi](i,j) = S(i,j) \tag{4.32}$$

where the Hermitian horizontal and vertical Helmholtz operators are defined by[6]

$$(\tilde{H}\phi)(i,j) = -\frac{1}{(\Delta z)^2}\left(\phi_{ij+1} + \phi_{ij-1} - 2\phi_{ij}\right) + \frac{1}{2a^2}\phi_{ij} \tag{4.33a}$$

$$(\tilde{V}\phi)(i,j) = -\frac{1}{(\Delta r)^2}\left(C_i\phi_{i+1,j} + C_{i-1}\phi_{i-1,j} - 2\phi_{ij}\right) + \frac{1}{2a^2}\phi_{ij} \tag{4.33b}$$

and

$$C_i = \frac{i}{\left(i^2 - \frac{1}{4}\right)^{1/2}} \tag{4.34}$$

The solution to Eqs. 4.33 is given iteratively by[79]

$$\phi^{m+\frac{1}{2}} = \frac{1}{(\tilde{H} + IR_{m+1})}\left[(IR_{m+1} - \tilde{V})\phi^m + S\right] \tag{4.35a}$$

$$\phi^{m+1} = \frac{1}{(\tilde{V} + IR_{m+1})}\left[(IR_{m+1} - \tilde{H})\phi^{m+\frac{1}{2}} + S\right] \tag{4.35b}$$

where I is the unit operator and the R_{m+1} are parameters chosen to accelerate the convergence. As in the case of Eqs. 4.14 and 4.15, the operator $\tilde{V}$ is represented by a matrix acting towards the right:

$$V_{i\ell} = \begin{cases} -C_{i-1}/(\Delta r)^2 & \ell = i-1 \\ 2/(\Delta r)^2 & \ell = i \\ -C_i/(\Delta r)^2 & \ell = i+1 \\ 0 & \text{elsewhere} \end{cases} \tag{4.36}$$

and the operator $\tilde{H}$ is represented by a matrix acting towards the left:

$$H_{\ell j} = \begin{cases} -1/(\Delta z)^2 & \ell = i \pm 1 \\ 2/(\Delta z)^2 & \ell = i \\ 0 & \text{elsewhere} \end{cases} \tag{4.37}$$

The matrices H and V are tridiagonal, so that the inversions may be performed rapidly by Gaussian elimination[38].

The optimal values of the acceleration parameters R_m for a two-step iteration are[6,79]

$$R_m = \begin{cases} \gamma - (\gamma^2 - \alpha\beta)^{1/2}, & m \text{ even} \\ \gamma + (\gamma^2 - \alpha\beta)^{1/2}, & m \text{ odd} \end{cases} \tag{4.38}$$

with $\gamma = (\alpha\beta)^{1/4}\left[\frac{1}{2}(\alpha+\beta)\right]^{1/2}$, α being the lower bound of the eigenvalues of H, β the upper bound of the eigenvalues of V.

From Eq. 4.33a, we see that $\tilde{H}$ is the discrete approximation to the operator

$$-\frac{\partial^2}{\partial z^2} + \frac{1}{2a^2}$$

The eigenfunctions of this operator are

$$\sin \frac{n\pi z}{(N_z-1)\Delta z}, \quad n = 1, 2, \ldots$$

and so the lower bound of the eigenvalues of H is

$$\alpha = \frac{\pi^2}{(N_z-1)^2(\Delta z)^2} + \frac{1}{2a^2} \tag{4.39}$$

Similarly Eq. 4.33b is the discrete approximation to the operator

$$-\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{2a^2} \tag{4.40}$$

The eigenfunctions of this operator are the Bessel functions of order 0

$$J_0\left(\frac{\alpha_{0n}\, r}{(N_R-\frac{1}{2})\,\Delta r}\right) \quad , \quad n = 1, 2, \ldots$$

where α_{0n} is the nth zero of J_0. As n increases $\alpha_{0n+1} - \alpha_{0n}$ rapidly approaches π. The eigenvalues of Eq. 4.40 are then approximated by

$$\frac{n^2\pi^2}{(N_R-\frac{1}{2})^2(\Delta r)^2} + \frac{1}{2a^2} \quad , \quad n = 1, 2, \ldots$$

However, since the matrix V is of dimension N_R, we have the further restriction that $n \leq N_R$. The upper bound of the eigenvalues of V is then

$$\alpha = \left(\frac{N_R}{N_R-\frac{1}{2}}\right)^2 \frac{\pi^2}{(\Delta r)^2} + \frac{1}{2a^2} \qquad (4.41)$$

Due to the short range of the Yukawa force, the boundary conditions for the Yukawa potential may be taken to be

$$U_{Yq}(i,1) = U_{Yq}(i,N_z) = U_{Yq}(N_R,j) = 0 \quad . \qquad (4.42)$$

The Coulomb potential is, however, a long range force and an explicit evaluation of Eq. 4.27 on the outer mesh edges becomes necessary. Performing the azimuthal integration, we obtain[49]

$$U_c(r,z) = 4e^2\int_0^{\infty} r'dr' \int_{-\infty}^{+\infty} dz' \, \frac{\rho(r',z')\,K(k)}{\left[(z-z')^2 + (r+r')^2\right]^{1/2}} \qquad (4.43)$$

where $K(k)$ is the complete elliptical

$$K(k) = \int_0^{\pi/2} \frac{dx}{(1 - k^2 \sin^2 x)^{1/2}} \tag{4.44}$$

and

$$k^2 = \frac{4rr'}{[(z-z')^2 + (r+r')^2]} \tag{4.45}$$

Eq. 4.44 is evaluated using the fourth degree polynomial approximation[81]

$$K(k) = [a_0 + a_1 m_1 + a_2 m_1^2 + a_3 m_1^3 + a_4 m_1^4] + [b_0 + b_1 m_1 + b_2 m_1^2 + b_3 m_1^3 + b_4 m_1^4] \ln(1/m_1) \tag{4.46a}$$

where

$$m_1 = 1 - m \tag{4.46b}$$

$$m = k^2 \tag{4.46c}$$

and

$a_0 =$ 1.38 629 436 112, $b_0 =$ .5

$a_1 =$ .09 666 344 259, $b_1 =$ .12 498 593 597

$a_2 =$ .03 590 092 383, $b_2 =$ .06 880 248 576

$a_3 =$ .03 742 563 713, $b_3 =$ .03 328 355 346

$a_4 =$ .01 451 196 213, $b_4 =$ .00 441 787 012

Eq. 4.43 is evaluated on the mesh edges by Simpson's rule:

$$U_c(i,j) = \frac{e^2}{r_i^{1/2}} \frac{2}{9} \Delta r \Delta z \sum_{i'=1}^{N_R-1} \sum_{j'=1}^{N_Z-1} \Big[f(i,j;i'+\tfrac{1}{2},j') + 2f(i,j;i',j') + 2f(i,j;i',j'+\tfrac{1}{2}) + 4f(i,j;i'+\tfrac{1}{2},j'+\tfrac{1}{2}) \Big] \tag{4.47a}$$

where

$$f(i,j;i',j') = k\, r_i^{1/2} K(k) \rho(i',j') \tag{4.47b}$$

4.3 Time Discretization

4.3.1 The Evolution Operator

Suppressing the spatial labels in Eq. 4.13, it can be written as

$$i\hbar \frac{\partial g_\alpha(t)}{\partial t} = (\tilde{H} + \tilde{V}) g_\alpha(t) \equiv \tilde{h}(t)\, g_\alpha(t) \tag{4.48}$$

where $\tilde{h}$ is Hermitian. Eq. 4.48 has the solution

$$g_\alpha(t) = U(t,t_0)\, g_\alpha(t_0) \tag{4.49}$$

where the time evolution operator is

$$U(t,t_0) = T \exp\left[\frac{-i}{\hbar} \int_{t_0}^{t} \tilde{h}(t')\,dt' \right] \tag{4.50}$$

and T is the Dyson time-ordering operator.

The time discretization is accomplished by defining the mesh[49]

$$t_n = n\,\Delta t \qquad , \quad n = 0, 1, 2, \ldots \qquad (4.51)$$

Eq. 4.50 can then be written in recursive form

$$g_\alpha^{(n+1)} = U(n+1, n)\, g_\alpha^{(n)} \qquad (4.52)$$

with $U(n+1,n) = U(t_{n+1}, t_n)$ and $g_\alpha^{(n)} = g_\alpha(t_n)$.

We approximate the evolution operator over the interval $[t_n, t_{n+1}]$ by the Peaceman-Rachford method[49,82]:

$$U(n+1,n) \approx \left[1 + \left(\frac{i\Delta t}{2\hbar}\right)\tilde{V}\right]^{-1}\left[1 - \left(\frac{i\Delta t}{2\hbar}\right)\tilde{H}\right] \times$$
$$\left[1 + \left(\frac{i\Delta t}{2\hbar}\right)\tilde{H}\right]^{-1}\left[1 - \left(\frac{i\Delta t}{2\hbar}\right)\tilde{V}\right] \qquad (4.53)$$

where $\tilde{H}$ and $\tilde{V}$ are defined by Eqs. 4.14 and 4.15. This expression approximates the time evolution operator through $\mathcal{O}(\Delta t)^2$. Since $\tilde{H}$ and $\tilde{V}$ are represented by tridiagonal matrices, (Eqs. 4.24 and 4.25), the inversions appearing in Eq. 4.53 can be performed rapidly by Gaussian elimination[38].

To solve Eq. 4.52, the time evolution is broken up into four steps[49]:

$$g_1^{(n)} = \left[1 - \left(\frac{i\Delta t}{2\hbar}\right)\tilde{V}\right] g^{(n)} \qquad (4.54a)$$

$$g_2^{(n)} = \left[1 + \left(\frac{i\Delta t}{2\hbar}\right)\tilde{H}\right]^{-1} g_1^{(n)} \qquad (4.54b)$$

$$g_3^{(n)} = \left[1 - \left(\frac{i\Delta t}{2\hbar}\right)\tilde{H}\right] g_2^{(n)} = 2\, g_2^{(n)} - g_1^{(n)} \qquad (4.54c)$$

$$g^{(n+1)} = \left[1 + \left(\frac{i\Delta t}{2\hbar}\right)\tilde{V}\right] g_3^{(n)} \qquad (4.54d)$$

4.3.2 The Construction of $\tilde{h}(t)$

In this subsection the method used to approximate $\tilde{h}(t)$ over the interval $[t_n, t_{n+1}]$ is discussed. Since the wave functions at t_{n+1} depend upon $\tilde{h}$, $\tilde{h}$ can only be specified in some implicit manner on the interval $[t_n, t_{n+1}]$. The simplest approximation is to take $\tilde{h} = \tilde{h}^{(n)}$, where $\tilde{h}^{(n)}$ is constructed at time t_n. This is known to give rise to serious violation of energy conservation[2], therefore the following construction of h is used[49]. We first construct

$$\bar{g}_\alpha = U^{(n)} g_\alpha^{(n)} \qquad (4.55)$$

where $U^{(n)}$ is defined by $\tilde{h}^{(n)}$ and Eq. 4.53. The average densities,

$$f = \tfrac{1}{2}\left(f^{(n)} + \bar{f}\right) \qquad (4.56)$$

where $f = \rho, \tau, j$ or s, are then used to define $\tilde{h}$ on the interval $[t_n, t_{n+1}]$.

4.4 The Static Hartree-Fock Problem

Static HF calculations are performed at time $t = 0$ in order to determine the starting wave functions. The energy functional used in the static HF calculations should be identical to the one used in the TDHF calculations. This is necessary so as to avoid unphysical oscillations of the nucleus when time dependent calculations are performed afterwards.

The static HF equations (Eq. 2.54) are solved using the imaginary time step technique[45]. This method is reportedly 50 times faster than the solutions found by the Lanczos method[28,49]. A further advantage provided by the imaginary time step technique is its invaluable aid in testing numerically the TDHF algorithm.

In section 4.4.1 we briefly discuss the conventional method of solving the static HF equations. The imaginary time step method is presented in section 4.4.2.

4.4.1 Usual Method of Solving the Static HF Equations

The most popular methods for solving the static HF equations are composed of four main steps[28,45]:

I) The single-particle orbitals are parametrized in a convenient fashion.

II) A physically reasonable approximation to the Hamiltonian, $\tilde{h}^{(0)}$, is made. The superscript here represents the iteration number.

III) The matrix elements of the Hamiltonian $\tilde{h}^{(n)}$ are then computed. A diagonalization of $\tilde{h}^{(n)}$ is performed to obtain simultaneously the single-particle wave functions $\psi_\alpha^{(n)}$ and the single-particle energies $\epsilon_\alpha^{(n)}$.

IV) The Hamiltonian $\tilde{h}^{(n+1)}$ is constructed from the wave functions determined in step III.

Steps III and IV are then iterated until convergence is achieved. A convenient measure of the stability of the eigenstates is the mean square deviation of the single-particle energies[45],

$$\Delta h^{(n)} = \sum_{\alpha} \left(\langle \psi_{\alpha}^{(n)} | \tilde{h}^{(n)2} | \psi_{\alpha}^{(n)} \rangle - \langle \psi_{\alpha}^{(n)} | \tilde{h}^{(n)} | \psi_{\alpha}^{(n)} \rangle^{2} \right)^{1/2} \quad (4.57)$$

Usually, $\Delta h^{(n)}$ is required to be less than 1 MeV, which results in an accuracy of 1% or better for the eigenvalues of the occupied states.

The parameterization mentioned in step I is usually accomplished either by expanding the wave functions in terms of a basis[83], or by discretizing the wave functions on a spatial mesh. For studies of light and medium mass nuclei, the parameterization is easily achieved by using an oscillator basis. However, for heavy deformed nuclei, such as the actinides, it is necessary to include up to 14 oscillator shells in the basis and even then the total energy is specified to an accuracy of 10 MeV[84]. Non-sparse matrices of the order of 100 x 100 must be handled, making the calculations very difficult. Furthermore, for shapes arising from heavy-ion collisions or fission, a usable oscillator basis is no longer adequate.

The discretization of the wave functions on a spatial mesh (section 4.2) avoids some of the problems generated by a basis expansion. A mesh size of 1 fm is usually sufficient to perform the static HF calculations. However, even with such a reasonable mesh size, large matrices are still needed. Their repeated diagonalization is very time consuming and inefficient. The imaginary time step technique provides a viable alternative.

4.4.2 Imaginary Time Step Technique

The imaginary time step technique consists of using the imaginary quantity $-i\Delta t$ in the TDHF equations. The wave functions of the TDHF equations then converge to the eigenstates of the static HF Hamiltonian, for sufficiently small Δt . The total energy will also monotonically decrease to the HF energy.

To show this, we consider the energy difference between two successive iterations (Eq. 2.44),

$$E^{(n+1)} - E^{(n)} = tr\left(\tilde{h}^{(n+\frac{1}{2})}\left(\rho^{(n+1)} - \rho^{(n)}\right)\right) \tag{4.58}$$

where $\tilde{h}^{(n+\frac{1}{2})}$ is a suitable approximation to $\tilde{h}$ on $[t_n, t_{n+1}]$ (section 4.3.2). If the wave functions are evolved according to

$$|\psi_\alpha^{(n+1)}\rangle = exp\left(\frac{-i}{\hbar}\Delta t\,\tilde{h}^{(n+\frac{1}{2})}\right)|\psi_\alpha^{(n)}\rangle \tag{4.59}$$

the one-body density matrix at time $(n+1)\Delta t$ is

$$\rho^{(n+1)} = exp\left(\frac{-i}{\hbar}\Delta t\,\tilde{h}^{(n+\frac{1}{2})}\right)\rho^{(n)} exp\left(\frac{+i}{\hbar}\Delta t\,\tilde{h}^{(n+\frac{1}{2})}\right) \tag{4.60}$$

From the cyclic invariance of the trace, Eq. 4.58 becomes

$$E^{(n+1)} - E^{(n)} = 0 \tag{4.61}$$

hence energy is conserved (section 2.4.4)

For an imaginary time step of the form $\Delta t = -i|\Delta t|$, Eq. 4.59 becomes

$$|\psi_\alpha^{(n+1)}\rangle = exp\left(-\lambda\tilde{h}^{(n+\frac{1}{2})}\right)|\psi_\alpha^{(n)}\rangle \tag{4.62}$$

where $\lambda = i\Delta t/\hbar$. In the limit of small λ , Eq. 4.62 can be approximated as

$$|\psi_\alpha^{(n+1)}\rangle = \left(1 - \lambda\tilde{h}^{(n+\frac{1}{2})}\right)|\psi_\alpha^{(n)}\rangle + \mathcal{O}(\lambda^2) \tag{4.63}$$

Orthonormalizing the wave functions using the Gram-Schmidt orthogonalization process, we obtain[45]

$$|\psi_\alpha^{(n+1)}\rangle = \left(1 - \lambda\left(\epsilon_{\alpha\alpha}^{(n)} - \tilde{h}^{(n+\frac{1}{2})}\right)\right)|\psi_\alpha^{(n)}\rangle + 2\lambda\sum_{\beta=1}^{\alpha-1} \epsilon_{\beta\alpha}^{(n)}\,|\psi_\beta^{(n)}\rangle + \mathcal{O}(\lambda^2) \tag{4.64}$$

where

$$\epsilon_{\beta\alpha}^{(n)} \equiv \langle\psi_\beta^{(n)}|\,\tilde{h}^{(n+\frac{1}{2})}\,|\psi_\alpha^{(n)}\rangle \tag{4.65}$$

Using Eq. 4.64 and the definition of the one-body density (Eq. 2.18), we obtain

$$\rho^{(n+1)} - \rho^{(n)} = -\lambda\left(\rho^{(n)}\tilde{h}^{(n+\frac{1}{2})}(1-\rho^{(n)}) + (1-\rho^{(n)})\tilde{h}^{(n+\frac{1}{2})}\rho^{(n)}\right) \tag{4.66}$$

The change in energy (Eq. 4.58) is then

$$E^{(n+1)} - E^{(n)} = -2\lambda\,\mathrm{tr}\left(\rho^{(n)}\tilde{h}^{(n+\frac{1}{2})}(1-\rho^{(n)})\tilde{h}^{(n+\frac{1}{2})}\right) \tag{4.67}$$

where the cyclic invariance of the trace was used. Defining the operator

$$A^{+} = \rho^{(n)}\tilde{h}^{(n+\frac{1}{2})}(1-\rho^{(n)}) \tag{4.68}$$

Eq. 4.67 becomes

$$E^{(n+1)} - E^{(n)} = -2\lambda\,\mathrm{tr}(A^{+}A) + \mathcal{O}(\lambda^2) \tag{4.69}$$

The energy is found to decrease after each iteration until the operator

A becomes zero. This gives the following condition

$$[\tilde{h}^{(n+\frac{1}{2})}, \rho^{(n)}]\rho^{(n)} = 0 \tag{4.70}$$

or equivalently

$$[\tilde{h}^{(n+\frac{1}{2})}, \rho^{(n)}] = \eta(1-\rho^{(n)}) \tag{4.71}$$

Using the idempotency of $\rho^{(n)}$, η is found to be zero. We then have the static HF equations.

In summary, for sufficiently small values of λ to justify the linear expansion (Eq. 4.63), the imaginary time step technique results in a monotonic decrease in the HF energy until the one-body density converges to the HF density. Moreover, the $\epsilon_{\beta\alpha}$ converge to zero for $\beta \neq \alpha$, and $\epsilon_{\alpha\alpha}$ converges to the eigenvalue corresponding to ψ_α.

4.5 Calculation of the Energies

4.5.1 The Total Energy

The total energy E is given by

$$E = \sum_{ij} \Delta V_i \,(H_0(i,j) + H_N(i,j) + H_V(i,j)) \tag{4.72}$$

where H_0, H_N, and H_V are given in Eqs. 4.11. The total energy can be broken up into 8 main parts:

- two-body local term

$$\sum_{ij} \Delta V_i \left\{ \tfrac{1}{2}\tilde{t}_0 \left[\left(1+\tfrac{\tilde{x}_0}{2}\right)\rho^2(i,j) - \left(\tfrac{1}{2}+\tilde{x}_0\right)\left(\rho_n^2(i,j)+\rho_p^2(i,j)\right)\right]\right\} \tag{4.73a}$$

- three-body local term

$$\sum_{ij} \Delta V_i \left\{ \frac{1}{4} t_3 \rho_n(i,j) \rho_p(i,j) \rho(i,j) \right\} \tag{4.73b}$$

- kinetic energy term

$$\sum_{ij} \Delta V_i \left\{ \frac{\hbar^2}{2m} \left(\tau_r(i+\tfrac{1}{2},j) + \tau_z(i,j+\tfrac{1}{2}) + s(i,j) \right) \right\} \tag{4.73c}$$

- effective mass contribution

$$\begin{aligned} \sum_{ij} \Delta V_i \Big\{ & \frac{t_1+t_2}{4} \left[\rho_z(i,j+\tfrac{1}{2}) \tau_z(i,j+\tfrac{1}{2}) + \rho(i,j) s(i,j) + \rho_r(i+\tfrac{1}{2},j) \tau_r(i+\tfrac{1}{2},j) \right] \\ & + \frac{t_2-t_1}{8} \sum_q \Big[\rho_{zq}(i,j+\tfrac{1}{2}) \tau_{zq}(i,j+\tfrac{1}{2}) + \rho_q(i,j) s_q(i,j) \\ & + \rho_{rq}(i+\tfrac{1}{2},j) \tau_{rq}(i+\tfrac{1}{2},j) \Big] \Big\} \end{aligned} \tag{4.73d}$$

- current density

$$\begin{aligned} \sum_{ij} \Delta V_i \Big\{ & \frac{t_1+t_2}{4} \left(j_z^2(i,j+\tfrac{1}{2}) + j_r^2(i+\tfrac{1}{2},j) \right) \\ & + \frac{t_2-t_1}{8} \sum_q \left(j_{zq}^2(i,j+\tfrac{1}{2}) + j_{rq}^2(i+\tfrac{1}{2},j) \right) \end{aligned} \tag{4.73e}$$

- Yukawa energy

$$\sum_{ij} \Delta V_i \, U_{Yq}(i,j) \tag{4.73f}$$

- Coulomb direct energy

$$\sum_{ij} \Delta V_i \, H_e^{(Dir)}(i,j) \tag{4.73g}$$

- Coulomb exchange energy

$$\sum_{ij} \Delta V_i \left\{ -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} e^2 \left[\rho_p(i,j)\right]^{1/3} \right. \tag{4.73h}$$

The following section deals with the single-particle energies.

4.5.2 Single-Particle Energies

In the Hartree-Fock approximation, the total energy for density-independent forces is given by

$$E = \frac{1}{2}\sum_{\alpha} n_\alpha (t_\alpha + \epsilon_\alpha) \tag{4.74}$$

where n_α is the occupation number of the α-th orbital, and t_α and ϵ_α denote the single-particle kinetic energies and single-particle energies respectively. It is not possible to obtain the radius, single-particle energies, and total binding energy of ^{16}O and ^{40}Ca if Eq. 4.74 holds[88].

For a density-dependent force of the Skyrme type, Eq. 4.74 is modified to

$$E = \frac{1}{2}\sum_{\alpha} n_\alpha (t_\alpha + \epsilon_\alpha) - \frac{1}{8} t_3 \int \rho_n \rho_p \rho \, d\vec{r} \tag{4.75}$$

We note that the binding energy of a nucleus is greater (with $t_3 > 0$) than what would be expected from Eq. 4.74. Vautherin and Brink[36] originally solved the static HF equations for the spherical closed shell nuclei, ^{16}O, ^{40}Ca, ^{90}Zr, and ^{208}Pb. They found several sets of parameters for the Skyrme force that reproduced the radii, single-particle energies, and total binding energies of these nuclei.

The total energy is also given by

$$E = \sum n_\alpha E_\alpha \tag{4.76}$$

where

$$E_\alpha = \langle \alpha | \frac{p^2}{2m} | \alpha \rangle + \frac{1}{2} \sum_{\beta} \langle \alpha\beta | \bar{v}_{12}^{(2)} | \alpha\beta \rangle + \frac{1}{6} \sum_{\beta\delta} \langle \alpha\beta\delta | \bar{v}_{123}^{(3)} | \alpha\beta\delta \rangle \tag{4.77}$$

The single-particle energy of the wave function ψ_α can then be expressed as

$$\epsilon_\alpha = 2 E_\alpha - t_\alpha + \frac{t_3}{4} \int \rho_q \rho n_\alpha | \psi_\alpha(\vec{r}) |^2 d\vec{r} \tag{4.78}$$

where $\alpha \epsilon q$. The energies E_α are found by the following equations:

$$\begin{aligned} E_\alpha = & \sum_{ij} f_{\rho_q}^{(\alpha)}(i,j) \Big\{ \frac{1}{2} \tilde{t}_0 \Big[(1 + \frac{\tilde{x}_0}{2}) \rho(i,j) - (\frac{1}{2} + \tilde{x}_0) \rho_q(i,j) \Big] \\ & + \frac{t_3}{4} \rho(i,j) \rho_q(i,j) + (V_\ell U_{Yp}(i,j) + V_\mu U_{Yn}(i,j)) \\ & + \delta_{qp} \Big(-\frac{3}{4} \Big(\frac{3}{\pi}\Big)^{1/3} e^2 \rho_p^{1/3}(i,j) \Big) \Big\} \\ & + \sum_{ij} f_{\tau_{zq}}^{(\alpha)}(i,j+\tfrac{1}{2}) \Big\{ \frac{\hbar^2}{2m} + \frac{t_1+t_2}{4} \rho_z(i,j+\tfrac{1}{2}) + \frac{t_2-t_1}{8} \rho_{zq}(i,j+\tfrac{1}{2}) \Big\} \\ & + \sum_{ij} f_{j_{zq}}^{(\alpha)}(i,j+\tfrac{1}{2}) \Big\{ -\frac{t_1+t_2}{4} j_z(i,j+\tfrac{1}{2}) - \frac{t_2-t_1}{8} j_{zq}(i,j+\tfrac{1}{2}) \Big] \\ & + \sum_{ij} f_{\tau_{rq}}^{(\alpha)}(i+\tfrac{1}{2},j) \Big\{ \frac{\hbar^2}{2m} + \frac{t_1+t_2}{4} \rho_r(i+\tfrac{1}{2},j) + \frac{t_2-t_1}{8} \rho_{rq}(i+\tfrac{1}{2},j) \Big\} \\ & + \sum_{ij} f_{s_q}^{(\alpha)}(i,j) \Big\{ \frac{\hbar^2}{2m} + \frac{t_1+t_2}{4} \rho(i,j) + \frac{t_2-t_1}{8} \rho_q(i,j) \Big\} \\ & + \sum_{ij} f_{j_{rq}}^{(\alpha)}(i+\tfrac{1}{2},j) \Big\{ -\frac{t_1+t_2}{4} j_r(i+\tfrac{1}{2},j) - \frac{t_2-t_1}{8} j_{rq}(i+\tfrac{1}{2},j) \Big\} \end{aligned} \tag{4.79}$$

where the probability densities are given by

$$f_{\rho_q}^{(\alpha)}(i,j) = 2\pi(\Delta r)^2\Delta z\,|g_\alpha(i,j)|^2 \tag{4.80a}$$

$$f_{s_q}^{(\alpha)}(i,j) = \frac{2\pi\Delta z}{(i-\frac{1}{2})^2}\,\mu_\alpha^2\,|g_\alpha(i,j)|^2 \tag{4.80b}$$

$$f_{\tau_{zq}}^{(\alpha)}(i,j+\tfrac{1}{2}) = \frac{2\pi(\Delta r)^2}{\Delta z}\,|g_\alpha(i,j) - g_\alpha(i,j+1)|^2 \tag{4.80c}$$

$$f_{j_{zq}}^{(\alpha)}(i,j+\tfrac{1}{2}) = 2\pi(\Delta r)^2\,\mathrm{Im}[g_\alpha^*(i,j)\,g_\alpha(i,j+1)] \tag{4.80d}$$

$$f_{\tau_{rq}}^{(\alpha)}(i+\tfrac{1}{2},j) = 2\pi\Delta z\left(\frac{i}{i-\frac{1}{2}}\right)\left|\left(\frac{i}{i-\frac{1}{2}}\right)^{1/2} g_\alpha(i,j) - \left(\frac{i}{i+\frac{1}{2}}\right)^{1/2} g_\alpha(i+1,j)\right|^2 \tag{4.80e}$$

$$f_{j_{rq}}^{(\alpha)}(i+\tfrac{1}{2},j) = 2\pi(\Delta r)(\Delta z)\left(\frac{i}{i-\frac{1}{2}}\right)\left(\frac{i}{i+\frac{1}{2}}\right)^{1/2}\mathrm{Im}[g_\alpha^*(i,j)\,g_\alpha(i+1,j)] \tag{4.80f}$$

4.6 Other Calculational Details

4.6.1 The Anisotropic Harmonic Oscillator

We use the anisotropic harmonic oscillator potential to describe the average nuclear field in the zero-th approximation:

$$h^{(0)} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \tag{4.81}$$

where the three frequencies ω_x, ω_y, and ω_z are chosen to be proportional to the inverse half axes of the ellipsoidal nucleus.

The condition of volume conservation is then

$$\omega_x\,\omega_y\,\omega_z \equiv \mathring{\omega}_0^3 = \text{constant} \tag{4.82}$$

$\dot{\omega}_0$ can be evaluated by using the special case of a spherical nucleus.

$$\hbar\dot{\omega}_0 = 41.43\,A^{-1/3}\ \mathrm{MeV} \tag{4.83}$$

For axially symmetric shapes, it is usual to introduce the deformation parameter δ :

$$\omega_\perp^2 \equiv \omega_x^2 = \omega_y^2 = \omega_0^2(\delta)\left(1+\tfrac{2}{3}\delta\right) \tag{4.84a}$$

$$\omega_z^2 = \omega_0^2(\delta)\left(1-\tfrac{4}{3}\delta\right) \tag{4.84b}$$

where

$$\omega_0(\delta) = \dot{\omega}_0\left[1-\tfrac{4}{3}\delta^2-\tfrac{16}{27}\delta^3\right]^{-1/6} \tag{4.84c}$$

The Hamiltonian (Eq. 4.81) is then

$$h^{(0)} = -\frac{\hbar^2}{2m}\left[\nabla^2 - \frac{m^2\omega_\perp^2}{\hbar^2}r^2 - \frac{m^2\omega_z^2}{\hbar^2}z^2\right] \tag{4.85}$$

and Schrodinger's equation

$$h^{(0)}\psi(r,z,\theta) = \epsilon\,\psi(r,z,\theta) \tag{4.86}$$

becomes

$$\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\partial^2}{\partial z^2} - \beta^2r^2 - \gamma^2z^2 + \frac{2m}{\hbar^2}\epsilon\right)\psi(r,z,\theta) = 0 \tag{4.87}$$

where $\beta = \dfrac{m\omega_\perp}{\hbar}$, $\alpha = \dfrac{m\omega_z}{\hbar}$ (4.88)

Using the method of seperation of variables, we find that the eigenfunctions of $h^{(0)}$ are

$$\Psi_{n_r m n_z}(r,\theta,z) = R_{n_r}^{|m|}(r)\,\Theta_m(\theta)\,Z_{n_z}(z) \tag{4.89a}$$

where

$$R_{n_r}^{|m|}(r) = \left[\frac{2\alpha\,(n_r!)}{(n_r+|m|)!}\right]^{1/2} e^{-\alpha r^2/2}\,(\sqrt{\alpha}\,r)^{|m|}\,L_{n_r}^{(|m|)}(\alpha r^2) \tag{4.89b}$$

$$n_r = 0, 1, 2, \ldots$$

$$\Theta_m(\theta) = \frac{1}{\sqrt{2\pi}}\,e^{-im\theta}\,, \qquad m = 0, \pm 1, \pm 2, \ldots \tag{4.89c}$$

$$Z_{n_z}(z) = \frac{\gamma^{1/4}}{[\sqrt{\pi}\,2^{n_z}\,n_z!]^{1/2}}\,e^{-\gamma z^2/2}\,H_{n_z}(\sqrt{\gamma}\,z) \tag{4.89d}$$

$$n_z = 0, 1, 2, \ldots$$

The $L_{n_r}^{(|m|)}$ are the Laguerre polynomials, and the H_{n_z} are the Hermite polynomials. Hence the eigenfunctions are characterized by the quantum numbers n_z , n_r , m, where m is the projection of the orbital angular momentum onto the symmetry axis. With

$$N = n_z + 2n_r + m_\ell \tag{4.90}$$

the corresponding energy eigenvalues are

$$\epsilon_{n_r m n_z} = \hbar\omega_z(n_z + \tfrac{1}{2}) + \hbar\omega_\perp(2n_r + m + 1) \tag{4.91a}$$

$$\approx \hbar\omega_0\left\{(N + \tfrac{3}{2}) + \delta\left(\frac{N}{3} - n_z\right)\right\} \tag{4.91b}$$

For $\delta = 0$, Eq. 4.91b becomes exact. Due to axial symmetry, m is a good quantum number.

4.6.2 Multipole Moments

For an axially symmetric system, the multipole operators $\hat{Q}_{\lambda 0}$ are given by

$$\hat{Q}_{\lambda 0} = r^{\lambda} Y_{\lambda 0}(\theta, \phi) \tag{4.92}$$

where $Y_{\lambda 0}$ are the spherical harmonics. In Eqs. 4.93, the quadrupole, octupole, and hexadecupole operators are given.

$$\hat{Q}_{20} = \sqrt{\frac{5}{16\pi}}\, r^{2} (3\cos^{2}\theta - 1) \tag{4.93a}$$

$$\hat{Q}_{30} = \sqrt{\frac{7}{16\pi}}\, r^{3} (5\cos^{3}\theta - 3\cos\theta) \tag{4.93b}$$

$$\hat{Q}_{40} = \sqrt{\frac{9}{256\pi}}\, r^{4} (35\cos^{4}\theta - 30\cos^{2}\theta + 3) \tag{4.93c}$$

The multipole operators are one-body operators and their expectation values are given by

$$Q_{\lambda 0} = \int \rho(\vec{r})\, r^{\lambda} Y_{\lambda 0}(\theta, \phi)\, d\vec{r} \tag{4.94}$$

To impose a set of multimoments on the nuclear system, we use the method of Lagrange multipliers. The new action to be minimized is

$$S + \sum_{\lambda} \alpha_{\lambda} (\langle \hat{Q}_{\lambda 0} \rangle - Q_{\lambda 0})^{2} \tag{4.95}$$

where α_{λ} and $Q_{\lambda 0}$ are parameters, and S is given by Eq. 4.12. The parameters $Q_{\lambda 0}$ are the multipole values desired to be imposed onto the nucleus. Upon taking the variation of Eq. 4.95 with respect to $g_{\alpha}^{*}(i,j)$

we find that the expression $h_{oq}(i,j)$ given in Eq. 4.16 has the additional term

$$\sum_{\lambda} \lambda \, \alpha_{\lambda} \left(\langle \hat{Q}_{\lambda o} \rangle - Q_{\lambda o} \right) \hat{Q}_{\lambda o} \qquad (4.96)$$

Chapter 5

RESULTS AND DISCUSSION

The imaginary time-step method is used to obtain the static Hartree-Fock solutions of ^{40}Ca for the axially symmetric case. In section 5.1 we present the results of the calculation.

5.1 Ground State Static HF Calculations for ^{40}Ca

We obtain the static HF solutions of the ground state of ^{40}Ca using the method outlined in Chapter 4. Due to computational considerations, we used a uniform mesh size of 1 fm with 7 mesh points in the radial direction and 15 mesh points in the direction of the z-axis. We found that a time step of 0.02 x 10^{-22} seconds provided reasonably fast convergence.

In order to determine the accuracy of the Coulomb and Yukawa iterative solutions, we evaluated numerically the Coulomb and Yukawa potentials for a spherical density distribution. The iteration scheme provided satisfactory values for the Yukawa potential but underestimated the values of the Coulomb potential. Iterative calculations of the Coulomb potential on a uniform mesh of 0.5 fm provided no significant improvement. We therefore found it necessary to evaluate the Coulomb potential numerically using Simpson's rule (section 4.2.3).

The convergence criterion for the HF solutions was taken to be that $\Delta h^{(n)} \leq 10$ MeV. This accuracy was achieved after 28 iterations using the double time-step method (section 4.3.2) for approximating $\tilde{h}^{(n+\frac{1}{2})}$. A total of 2954 S.R.U.'s of computer time on a CDC Cyber-170 was needed for the run.

The neutron and proton density profiles are shown in Fig. 1 and Fig. 2. Table II shows the calculated values of r.m.s. radius of the nucleus (r_m), neutrons (r_n), protons (r_p), charge distribution (r_c) and of the binding energy per particle for ^{40}Ca. Corrections to the nuclear-charge distribution to allow for the finite extent of the proton-charge distribution were done using the proton form factor[36].

$$f_p(\vec{r}) = \frac{1}{(r_0\sqrt{\pi})^3}\, e^{-r^2/r_0^2} , \qquad r_0 = 0.65 \text{ fm}$$

The charge distribution $\rho_c(\vec{r})$ is obtained by folding this form factor with the proton density distribution $\rho_p(\vec{r})$

$$\rho_c(\vec{r}) = \int f_p(\vec{r}-\vec{s})\, \rho_p(\vec{s})\, d\vec{s} .$$

The calculated r.m.s. agree reasonably well with those obtained by Vautherin and Brink[36], The r.m.s. radius of the charge distribution is in agreement with the experimental value of 3.49 fm.

The calculated binding energy per particle however, is about 2 MeV lower than the value obtained by Vautherin and Brink, and the experimental value. In Table IV, a detailed breakdown of the various contributions to the nuclear binding energy is compared to the results obtained by Hoodboy and Negele[28]. The 2-body zero range term and the Coulomb terms are in agreement. The magnitude of the other terms are however in strong disagreement. We attribute the difference in the energies mainly to the mesh size difference - Hoodboy and Negele used a mesh size of 0.40 fm while we used a mesh size of 1 fm. Static HF calculations in rectangular coordinates done by Davies et al[45], using a mesh size of 1 fm, gave a binding energy of -307.656 MeV for ^{40}Ca. The parameters in Table I need to be adjusted for large mesh size.

The single-particle energies are shown in Table III. Considering the omission of the spin-orbit force, the values that were obtained for the single-particle energies agree reasonably well with the energy levels obtained by Vautherin and Brink.

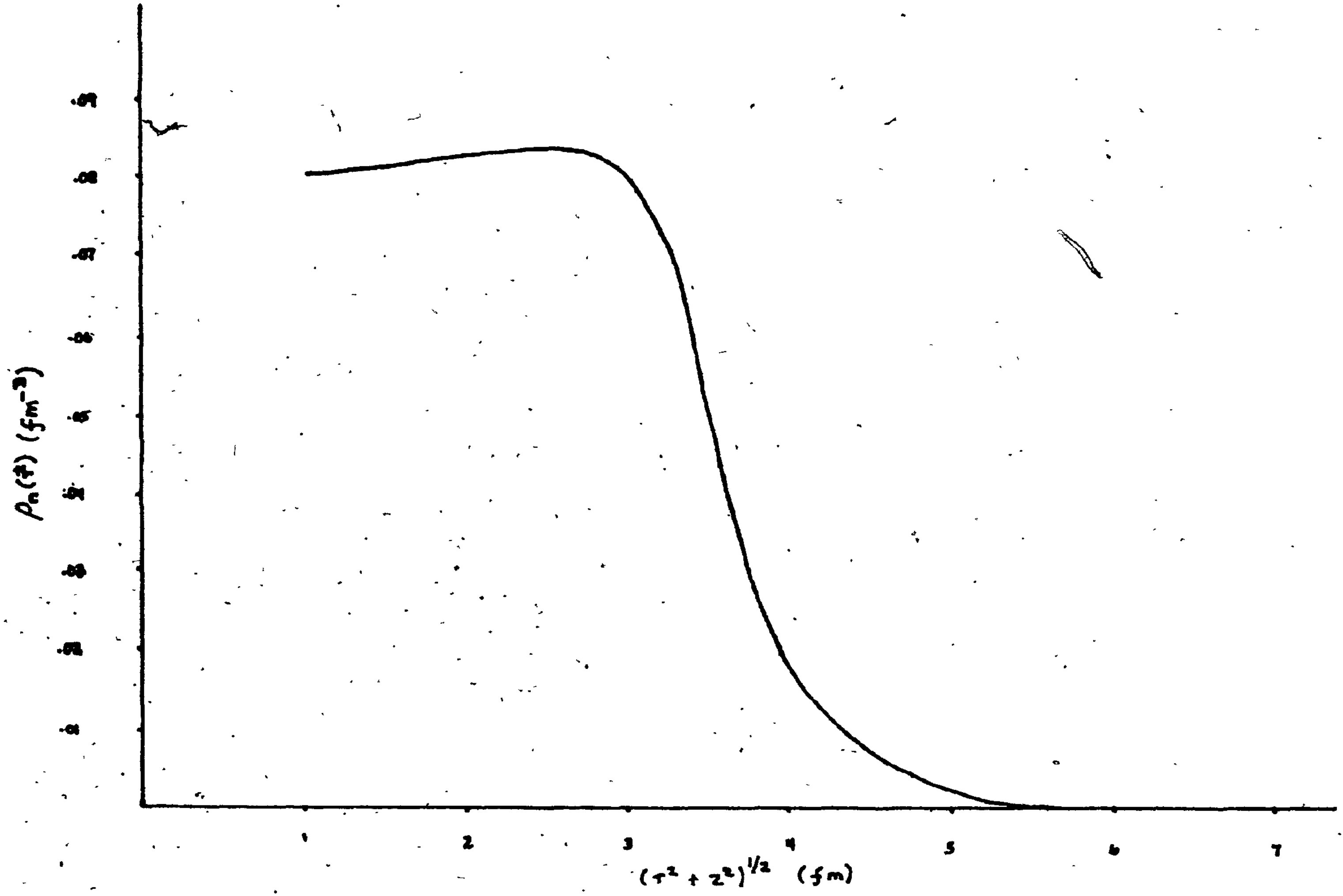

Fig. 1. Neutron density distribution of ^{40}Ca using the parameters in Table I.

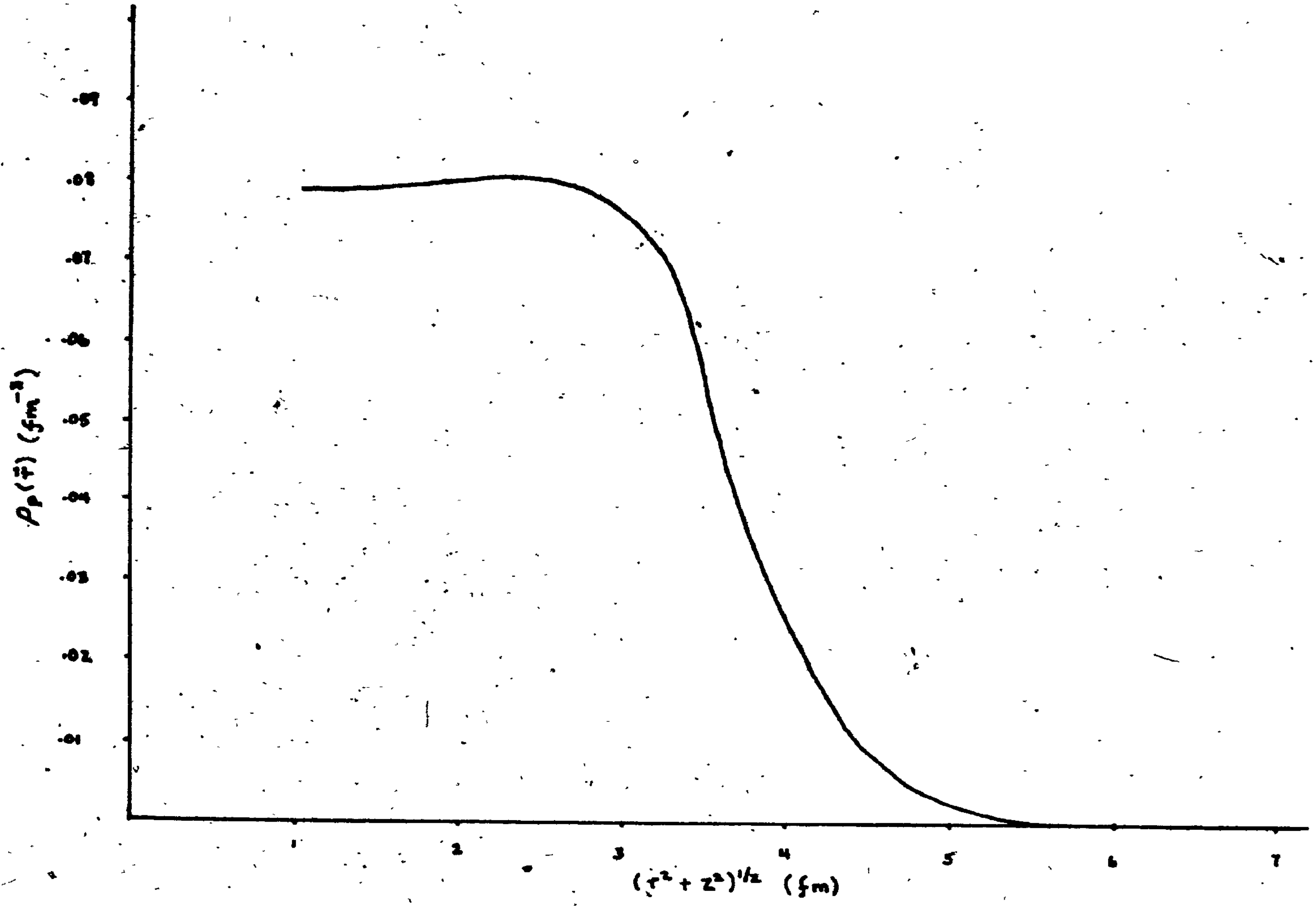

Fig. 2. Proton density distribution of ^{40}Ca using the parameters in Table I.

TABLE II. Root mean square radii (fm) and total binding energy per particle (MeV) obtained for ^{40}Ca are compared with the values obtained by Vautherin and Brink[36] in column 2.

r_m	3.25	3.38
r_n	3.23	3.35
r_p	3.26	3.40
r_c	3.36	3.49
E/A	-6.62	-8.41

TABLE III. Occupied single-particle energies (MeV) obtained for ^{40}Ca are compared with the values obtained by Vautherin and Brink[36].

	NEUTRONS			PROTONS		
	computed		Ref. 36	computed		Ref. 36
1s	-44.93	$1s_{1/2}$	-55.33	-33.34	$1s_{1/2}$	-47.11
1p	-36.13	$1p_{3/2}$	-39.22	-28.89	$1p_{3/2}$	-31.30
	-32.43	$1p_{1/2}$	-36.08	-25.09	$1p_{1/2}$	-28.30
1d	-24.73	$1d_{5/2}$	-23.26	-17.69	$1d_{5/2}$	-15.67
	-21.67			-14.62		
	-19.49	$1d_{3/2}$	-17.53	-12.44	$1d_{3/2}$	-10.10
2s	-13.21	$2s_{1/2}$	-17.08	- 6.35	$2s_{1/2}$	- 9.57

TABLE IV. A detailed breakdown of the various contributions to the nuclear binding energy of ^{40}Ca. These values are compared with the results obtained by Hoodboy and Negele[28] in column 2.

Kinetic energy	791.558	688.846
Effective mass contribution	418.389	346.314
2-body zero range	-188.264	-172.525
3-body zero range	400.507	338.419
Yukawa	-1760.103	-1631.836
Coulomb (exchange)	-7.990	-7.736
Coulomb (direct)	80.760	81.592
	-265.143	-356.926

Chapter 6

CONCLUSIONS

Static Hartree-Fock calculations have been performed successfully for ^{40}Ca using the imaginary time step method. The results obtained agree reasonably well with the spherical calculations performed by Vautherin and Brink and the axially symmetric calculations performed by Hoodboy and Negele using the Lanczos algorithm. The larger binding energies that we obtained are mainly due to the neglect of the spin-orbit force which would give a negative contribution to the total binding energy.

It was found that the iterative scheme outlined in section 4.2.3 gave very satisfactory results for the evaluation of the Yukawa potential. However, the iterative scheme underestimated the Coulomb potential. It was necessary to evaluate the Coulomb potential numerically at each point of the mesh.

This work lays the foundations for future microscopic calculations. The present program, being written in the interactive programming language APL, can readily be extended to describe nuclear structure, fission phenomena, and heavy ion nuclear collisions. A research problem for the future will be to modify the TDHF equations in a suitable way so as to permit the nuclear system to undergo transitions from one energy surface to another. This can be accomplished by including some time-dependence into the occupation numbers n_α. One method of obtaining time dependent occupation numbers consists of imposing the condition that at each instant in time the lowest energy levels are filled so that as two distinct energy levels cross, a pair of nucleons jump from one level to the other. However, the stability of these modified TDHF solutions should be examined first.

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APPENDIX A

The Computer Program

Due to the complexity of the algorithm, we found it best to write the program in APL[89]. APL is an interactive computer language. This permitted us to easily follow and analyze each step of the program run. The functions in Table A which have no asterix are listed on the subsequent pages. The functions marked with an asterix are locked functions and were copied from *APL1 FILESYS. A listing for these functions is not available.

TABLE A. List of the functions used for the Hartree-Fock calculations.

BCCOUL	COMPARE	COPYF	COULOMB	COUL1	CREATEF	DENHO
DENS	DENSITY	DETK	DISFNS	DISVARS	ENCONV	ENERGY
ENERGYT	ENERN	ENERP	ENORDER	EPORDER	ERASEV	ERLOCK
EVOLVEN	EVOLVEP	FCREATE*	FERASE*	FNAMES*	FNUMS*	FREAD*
FSAVE	FTIE*	FUNTIE*	FWRITE*	GOIF	GRAM	GRAMSCH
HALFDEN	INITIAL	LIST	LISTFNS	MAINORM	MPFIXL	MPMEAS
MPTERMS	NORM	NORMAIN	NORMDEN	NUCMAT	PHI	PHIT
PLOTRAD	QUANTO	RADIAL	REC26	REC32	REC33	REC34
RMSRAD	SAVEF	SDENHO	SEEDENS	SEEFILE	SEEWF	SETNOS
SETYC	SPACE	STDHF	STODENS	SUMDENS	TDENS	TERMS
TIEF	UNTIEF	WAIT	WFN	WFNORM	YUKAWA	ZED

```
    ∇ BCCOUL;P00;P01;P10;P11;M01;M10;M11;M00;I11;I00;J00;J11
[ 1]  SPACE2
[ 2]  '  ENTERING BCCOUL'
[ 3]  P00←0 1↓¯1 ¯1↓PP
[ 4]  P01←¯1 0↓PZP
[ 5]  P10←0 1↓0 ¯1↓PRP
[ 6]  P11←0.5×(0 1↓PRP)+0 ¯1↓PRP
[ 7]  T←DZ÷DR
[ 8]  M01←⍉((NZT-1),NR-1)⍴I00←¯0.5+⍳NR-1
[ 9]  M00←0 1↓M01
[10]  M11←0.5+M01
[11]  M10←0 1↓M11
[12]  I11←0.5+I00
[13]  J00←1+⍳NZT-2
[14]  J11←0.5+⍳NZT-1
[15]  C←2×DR×DZ×1.4399763÷9
[16]  A←FREAD 11 17
[17]  B←FREAD 11 18
[18]  BCD←(NZT)⍴BCL←BCR←(NR-1)⍴0
[19]  IP←1
[20] L1:BCL[IP]←PHI(IP,1)
[21]  BCR[IP]←PHI(IP,NZT)
[22]  →L1×⍳NR>IP←IP+1
[23]  JP←1
[24] L2:BCD[JP]←PHI(NR,JP)
[25]  →L2×⍳NZT≥JP←JP+1
[26]  BCL←BCL,BCD[1]
[27]  BCR←BCR,BCD[NZT]
[28]  BCL FWRITE 11 19
[29]  BCR FWRITE 11 20
[30]  BCD FWRITE 11 21
[31]  '  LEAVING BCCOUL'
[32]  SPACE2
    ∇
```

```
    ∇ COMPARE;A;B;C
[ 1]  TEMC←TENEMCP+TENEMCN
[ 2]  TYU←TENYUP+TENYUN
[ 3]  T2B←TEN2BP+TEN2BN
[ 4]  T3B←TEN3BP+TEN3BN
[ 5]  T3←TE3P+TE3N
[ 6]  T46←TE46P+TE46N
[ 7]  T57←TE57P+TE57N
[ 8]  T8←TE8N+TE8P
[ 9]  T911←TE911P+TE911N
[10]  T1012←TE1012N+TE1012P
[11]  THD←THDP+THDN
[12]  THH←THHP+THHN
[13]  THV←THVP+THVN
[14]  TENTOT←TENTOTN+TENTOTP
[15]  TENSP←TENSPN+TENSPP
[16]  TCUR←TENCURP+TENCURN
```

```
[17]  TKE←TENKEF+TENKEN
[18]  THF←0.5×TKE+TENTOT-T3B
[19]  THF2←0.5×TKE+TEMC+TENTOT-T3B
[20]  TFE←TENTOT-TKE
[21]  A46←E4+E6
[22]  A57←E5+E7
[23]  A911←E9+E11
[24]  A1012←E10+E12
[25]  B←EOLD,TENTOTN,TENTOTF,TENTOT,TYU,T2B,T3B,TKE,TCUR
[26]  B←B,TEMC,TENCD,TENCE,T3,T46,T57,T8,T911,T1012
[27]  B←B,THO,THH,THV,TENSF,THF2,TFE
[28]  B←B,0,0,ENTOTAL,ENYU,EN2B,EN3B,ENKE,ENCUR
[29]  B←B,ENEMC,ENCD,ENCE,E3,A46,A57,E8,A911
[30]  B←B,A1012,HO,HH,HV,ENSF,THF2,TFE
[31]  B←⍉3 23⍴B
[32]  C←'F13.3'⎕FRMT B
[33]  SPACE2
[34]  ⎕←(39⍴' '),'    OLD S.P.         NEW S.P.           TOTAL'
[35]  SPACE1
[36]  A←FREAD 11 26
[37]  (A,C)FWRITE(3,ITIME)
[38]  ⎕←A,C
[39]  WAIT
[40]  SPACE2
    ∇


     ∇ TNEW COPYF TOLD;A;B;I;C
[1]   SPACE1
[2]   I←0
[3] L1:A←FREAD(TOLD,I)
[4]   A FWRITE(TNEW,I)
[5]   →L1×⍳IM≥I←I+1
[6]   'LAST RECORD COPIED IS ';I-1
[7]   SPACE1
     ∇


     ∇ COULOMB;P00;P01;P10;P11;M01;M10;M11;M00;I11;I00;J00;J11
[ 1]  SPACE2
[ 2]  'ENTERING COULOMB'
[ 3]  P00←0 1↓¯1 ¯1↓PP
[ 4]  P01←¯1 0↓PZP
[ 5]  P10←0 1↓0 ¯1↓PRP
[ 6]  P11←0.5×(0 1↓PRP)+0 ¯1↓PRP
[ 7]  T←DZ÷DR
[ 8]  M01←⍉((NZT-1),NR-1)⍴I00←¯0.5+⍳NR-1
[ 9]  M00←0 1↓M01
[10]  M11←0.5+M01
[11]  M10←0 1↓M11
[12]  I11←0.5+I00
[13]  J00←1+⍳NZT-2
```

```
[14]  J11←0.5+⍳NZT-1
[15]  C←2×DR×DZ×1.4399763÷9
[16]  A←FREAD 11 17
[17]  B←FREAD 11 18
[18]  BCD←(NZT)⍴BCL←BCR←(NR-1)⍴0
[19]  UCP←PP×0
[20]  IP←1
[21] L1:BCL[IP]←PHI(IP,1)
[22]  BCR[IP]←PHI(IP,NZT)
[23]  →L1×⍳NR>IP←IP+1
[24]  JP←1
[25] L2:BCD[JP]←PHI(NR,JP)
[26]  →L2×⍳NZT≥JP←JP+1
[27]  BCL←BCL,BCD[1]
[28]  BCR←BCR,BCD[NZT]
[29]  UCP[NR;]←BCD
[30]  UCP[;1]←BCL
[31]  UCP[;NZT]←BCR
[32]  IP←1
[33] L3:JP←2
[34] L4:UCP[IP;JP]←PHI(IP,JP)
[35]  →L4×⍳NZT>JP←JP+1
[36]  →L3×⍳NR>IP←IP+1
[37]  RIH←⍉(NZT,NR)⍴(DR×¯0.5+⍳NR)*0.5
[38]  UCP←UCP÷RIH
[39]  'LEAVING COULOMB'
[40]  SPACE2
    ∇


    ∇ COUL1;S;AA;BB;RIH;M;ML;R0;R1;R2;R3;R4;R5;R6;R7;Z;N
[ 1]  SPACE3
[ 2]  '  ENTERING COULOMB FUNCTION'
[ 3]  R0←FREAD 11 8
[ 4]  R1←FREAD 11 9
[ 5]  R2←FREAD 11 10
[ 6]  R3←FREAD 11 11
[ 7]  R4←FREAD 11 12
[ 8]  R5←FREAD 11 13
[ 9]  R6←FREAD 11 14
[10]  R7←FREAD 11 15
[11]  RIH←⍉(NZT,NR)⍴(DR×¯0.5+⍳NR)*0.5
[12]  M←0
[13]  S←RIH×PP×4×1.4399763×○1
[14]  AA←PP
[15]  →L1×⍳ITIME=0
[16]  UCP←FREAD(201,ITIME-1)
[17]  AA←RIH×UCP
[18]  ML←6
[19]  →L3×⍳4>CFLAG←CFLAG+1
[20] L1:BCCOUL
[21]  AA[;1]←BCL
[22]  AA[;NZT]←BCR
```

```
[23]  AA[NR;]←BCD
[24]  CFLAG←0
[25]  →L3×⍳ITIME≠0
[26]  AA←BCR∘.+BCD
[27]  AA[;1]←AA[;NZT]←BCR
[28]  AA[NR;]←BCD
[29]  ML←20
[30] L3:' SUGGESTED NO. OF ITERATIONS IS  ';ML
[31]  Z←|AA
[32]  N←' AA '
[33]  M←0
[34] L4:BB←(S+R1+.×AA)+.×R7
[35]  AA←R5+.×(S+BB+.×R3)
[36]  BB←(S+R0+.×AA)+.×R6
[37]  AA←R4+.×(S+BB+.×R2)
[38]  AA[;1]←BCL
[39]  AA[;NZT]←BCR
[40]  AA[NR;]←BCD
[41]  M←M+2
[42]  NORM AA
[43]  →L4×GOIF'Y'
[44]  UCP←AA÷RIH
[45]  UCP FWRITE(201,ITIME)
[46]  'LEAVING COULOMB FUNCTION'
[47]  SPACE3
    ∇


    ∇  CREATEF;M;N;D;I
[ 1]  M←FREAD 11 24
[ 2]  N←FREAD 11 25
[ 3]  D←(⍴M)[1]
[ 4]  I←1
[ 5] L1:M[I;]FCREATE N[I]
[ 6]  →L1×⍳D≥I←I+1
[ 7]  N←((⍴FNUMS),1)⍴FNUMS
[ 8]  'THE FOLLOWING ARE THE FILES THAT ARE NOW TIED'
[ 9]  '    '
[10]  FNAMES,⍕N
    ∇


    ∇  X DENHO A;NR1;NZ1;N
[ 1]  A←A[1;;]
[ 2]  →L1×⍳I≠1
[ 3]  PP←PN←SP←SN←(NR,NZT)⍴0
[ 4]  NR1←NR-1
[ 5]  NZ1←NZT-1
[ 6]  TZP←TZN←JZP←JZN←(NR,NZ1)⍴0
[ 7]  TRP←TRN←JRP←JRN←(NR1,NZT)⍴0
[ 8] L1:→L2×⍳X=3
[ 9]  N←OCCP[I]
```

```
[10]  PP←PP+N×A*2
[11]  TZP←TZP+(0 ¯1↓A)×(0 1↓A)×N
[12]  TRP←TRP+(¯1 0↓A)×(1 0↓A)×N
[13]  SP←SP+(MP[I]*2)×(A*2)×N
[14]  →0×⍳X=2
[15] L2:N←OCCN[I]
[16]  PN←PN+N×A*2
[17]  TZN←TZN+(0 ¯1↓A)×(0 1↓A)×N
[18]  TRN←TRN+(¯1 0↓A)×(1 0↓A)×N
[19]  SN←SN+(MN[I]*2)×(A*2)×N
    ∇


    ∇ PTN DENS NTN;ALPHA;G
[ 1]  SPACE1
[ 2]  'ENTERING DENS'
[ 3]  ALPHA←1
[ 4] L1:G←FREAD(PTN,ALPHA)
[ 5]  1 DENSITY G
[ 6]  →L1×⍳NMP≥ALPHA←ALPHA+1
[ 7]  ALPHA←1
[ 8] L2:G←FREAD(NTN,ALPHA)
[ 9]  2 DENSITY G
[10]  →L2×⍳NMN≥ALPHA←ALPHA+1
[11]  SUMDENS
[12]  TDENS
[13]  'LEAVING DENS'
[14]  SPACE1
    ∇


    ∇ X DENSITY A;RG;IG;P;TZ;TR;JZ;JR;N;M
[ 1]  RG←A[1;;]
[ 2]  IG←A[2;;]
[ 3]  P←(RG*2)+IG*2
[ 4]  TZ←((0 ¯1↓RG)×(0 1↓RG))+(0 ¯1↓IG)×0 1↓IG
[ 5]  TR←((¯1 0↓RG)×(1 0↓RG))+(¯1 0↓IG)×1 0↓IG
[ 6]  JZ←((0 ¯1↓RG)×(0 1↓IG))-(0 ¯1↓IG)×0 1↓RG
[ 7]  JR←((¯1 0↓RG)×(1 0↓IG))-(¯1 0↓IG)×1 0↓RG
[ 8]  →L2×⍳X=1
[ 9]  →L3×⍳ALPHA=1
[10] L1:N←OCCN[ALPHA]
[11]  M←MN[ALPHA]
[12]  PN←PN+N×P
[13]  SN←SN+P×N×M×M
[14]  TZN←TZN+N×TZ
[15]  TRN←TRN+N×TR
[16]  JZN←JZN+N×JZ
[17]  JRN←JRN+N×JR
[18]  →0
[19] L2:→L4×⍳ALPHA=1
[20] L5:N←OCCP[ALPHA]
```

```
[21]  M←MP[ALPHA]
[22]  PP←PP+N×P
[23]  SP←SP+P×N×M×M
[24]  TZP←TZP+N×TZ
[25]  TRP←TRP+N×TR
[26]  JZP←JZP+N×JZ
[27]  JRP←JRP+N×JR
[28]  →0
[29] L3:PN←SN←(NR,NZT)⍴0
[30]  TZN←JZN←0 1↓PN
[31]  TRN←JRN←1 0↓PN
[32]  →L1
[33] L4:PP←SP←(NR,NZT)⍴0
[34]  TZP←JZP←0 1↓PP
[35]  TRP←JRP←1 0↓PP
[36]  →L5
    ∇
```

```
   ∇  K←DETK M
 [1]  K←-(B[1]+M×B[2]+M×B[3]+M×B[4]+M×B[5])×⍟M←1-M
 [2]  K←K+A[1]+M×A[2]+M×A[3]+M×A[4]+M×A[5]
   ∇
```

```
   ∇  DISFNS;MAT;L;LL
 [1]  MAT←⎕NL 3
 [2]  R←(⍴MAT)[1]
 [3]  L←⌈R÷7
 [4]  LL←L×7
 [5]  MAT←(LL,9)↑MAT
 [6]  MAT←(L,¯73)↑(L,63)⍴MAT
 [7]  MAT
   ∇
```

```
   ∇  DISVARS;MAT;L;LL
 [1]  MAT←⎕NL 2
 [2]  R←(⍴MAT)[1]
 [3]  L←⌈R÷7
 [4]  LL←L×7
 [5]  MAT←(LL,9)↑MAT
 [6]  MAT←(L,¯73)↑ (L,63)⍴MAT
 [7]  MAT
   ∇
```

```
   ∇  ENCONV
 [1]  SPACE1
 [2]  'AT ITIME=  ';ITIME
```

```
      SPACE1
      'OLD DELTA OF SINGLE PARTICLE-ENERGIES IS ....... ';DELENO
      DELENO←DELENN+DELENP
      'NEW DELTA OF SINGLE PARTICLE-ENERGIES IS ....... ';DELENO
      SPACE1
    ∇
```

```
    ∇  TN ENERGY TP;I;IS;IT1;IT2;IT4;IJ;AA;BB;B1;IT5
       SPACE2
       ' ENTERING ENERGY'
       CP←DR×DR×DZ×○2
       CTZ←DR×DR×(○2)÷DZ
       CJZ←DR×DR×○2
       CS←CTR←DZ×○2
       CJR←DR×DZ×○2
       IS←1÷(¯0.5+I←⍉(NZT,NR)⍴⍳NR)*2
       IT1←(2,⍴IT4)⍴(IT4←¯1 0↓IT5←I÷I-0.5)*0.5
       IT2←(2,⍴IJ)⍴IJ←¯1 0↓(I÷I+0.5)*0.5
       A←FREAD 11 22
       B←FREAD 11 23
       KQ←B[2]+B[3]
       KNQ←B[2]÷KQ
       B1←B[1]
       →L10×⍳ITIME=0
       EOLD←TENTOTN,TENTOTP,TENTOT,TYU,T2B,T3B,TKE,TCUR
       EOLD←EOLD,TEMC,TENCD,TENCE,T3,T46,T57,T8
       EOLD←EOLD,T911,T1012,THO,THH,THV,THF,THF2,TPE
       →L15
      L10:EOLD←23⍴0
      L15:SPACE2
       ENERN TN
       ENERN TP
       COMPARE
    ∇
```

```
    ∇  ENERGYT;DV;DVR;DVZ;A;B;P;JR;JZ;PZ;PR;DZM2;DRM2;C
       A←FREAD 11 22
       B←FREAD 11 23
       DV←(DR×DR×DZ×○2)×⍉(NZT,NR)⍴¯0.5+⍳NR
       DVZ←0 ¯1↓DV
       DVR←(DR×DR×DZ×○1)+¯1 0↓DV
       P←PP+PN
       JR←JRP+JRN
       JZ←JZP+JZN
       PZ←PZP+PZN
       PR←PRP+PRN
       DZM2←1÷DZ×DZ
       DRM2←1÷DR×DR
       ENCD←0.5×+/,PP×UCP×DV
       ENCE←-0.75×A[6]×+/,DV×PP*4÷3
```

```
[15]  ENYU←0.5×+/,DV×(A[5]×(PN×UYN)+PP×UYP)+A[4]×(PN×UYP)+PP×UYN
[16]  EN2B←0.5×+/,DV×(A[1]×P×P)-A[2]×(PN×PN)+PP×PP
[17]  EN3B←A[3]×+/,DV×P×PN×PP
[18]  E3←RAW×2×DZM2×B[1]×+/,DVZ×TZN+TZP
[19]  E4←2×DZM2×B[2]×+/,DVZ×PZ×TZN+TZP
[20]  E5←-DZM2×B[2]×+/,DVZ×JZ×JZ
[21]  E6←2×DZM2×B[3]×+/,DVZ×(PZN×TZN)+PZP×TZP
[22]  E7←-DZM2×B[3]×+/,DVZ×(JZN×JZN)+JZP×JZP
[23]  E8←RAW×DRM2×B[1]×(2×+/,DVR×TRN+TRP)++/,DV×SN+SP
[24]  E9←DRM2×B[2]×(2×+/,DVR×PR×TRN+TRP)++/,DV×P×SN+SP
[25]  E10←-DRM2×B[2]×+/,DVR×JR×JR
[26]  E11←DRM2×B[3]×(2×+/,DVR×(PRN×TRN)+PRP×TRP)++/,DV×(PN×SN)+PP×SP
[27]  E12←-DRM2×B[3]×+/,DVR×(JRN×JRN)+JRP×JRP
[28]  ENKE←E3+E8
[29]  ENEMC←E4+E6+E9+E11
[30]  ENCUR←E5+E7+E10+E12
[31]  HO←EN2B+EN3B+ENCE+ENCD+ENYU
[32]  HV←E8+E9+E10+E11+E12
[33]  HH←E3+E4+E5+E6+E7
[34]  ENTOTAL←HO+HV+HH
[35]  ENSP←(2×ENTOTAL)+EN3B-ENKE
[36]  B←0.5×ENKE+ENEMC+ENTOTAL-EN3B
[37]  C←ENTOTAL-ENKE
[38]  'TOTAL ENERGY ............................. ';ENTOTAL
[39]  'TOTAL SINGLE-PARTICLE ENERGY ............. ';ENSP
[40]  'TOTAL HARTREE-FOCK ENERGY WITH EMC ........ ';B
[41]  'TOTAL POTENTIAL ENERGY .................... ';C
[42]  SPACE2
    ∇


    ∇ ENERN TN;MYU;M2B;M3B;M46;M57;M911S;M911P;M1012;F;GP;GM;MCE
[ 1]  SPACE1
[ 2]  'ENTERING ENERN'
[ 3]  ENYUN←EN2BN←EN3BN←E3N←E46N←E57N←E8N←E911N←E1012N←NMN⍴0
[ 4]  MYU←0.5×(A[5]×UYN)+A[4]×UYP
[ 5]  M2B←0.5×(PN×A[1]-A[2])+A[1]×PP
[ 6]  M3B←0.5×A[3]×PP×PN+PP
[ 7]  M46←(2÷DZ×DZ)×KQ×TZN+KNQ×TZP
[ 8]  M57←(¯1÷DZ×DZ)×KQ×JZN+KNQ×JZP
[ 9]  M911S←(1÷DR×DR)×KQ×SN+KNQ×SP
[10]  M911P←KQ×PRN+KNQ×PRP
[11]  M1012←(¯1÷DR)×KQ×JRN+KNQ×JRP
[12]  ALPHA←1
[13] L1:G←FREAD(TN,ALPHA)
[14]  F←CP×+/[1]G×G
[15]  ENYUN[ALPHA]←+/,F×MYU
[16]  EN2BN[ALPHA]←+/,F×M2B
[17]  EN3BN[ALPHA]←+/,F×M3B
[18]  E911N[ALPHA]←+/,F×M911S
[19]  GP←0.5×(0 1↓F)+0 ¯1↓F
[20]  E46N[ALPHA]←+/,GP×M46
[21]  GP←0 0 1↓G
```

```
[22]   GM←0 0 ¯1↓G
[23]   F←CJZ×(GM[1;;]×GP[2;;])-GM[2;;]×GP[1;;]
[24]   E57N[ALPHA]←+/,F×M57
[25]   F←CTZ×+/[1]F×F←GM-GP
[26]   E3N[ALPHA]←B[1]×+/,F
[27]   F←(CS×MN[ALPHA]*2)×+/[1]G×G
[28]   E8N[ALPHA]←B[1]×+/,F×IS
[29]   GP←0 1 0↓G
[30]   GM←0 ¯1 0↓G
[31]   F←CTR×IT4×+/[1]F×F←(IT1×GM)-IT2×GP
[32]   E8N[ALPHA]←E8N[ALPHA]+B[1]×+/,F
[33]   E911N[ALPHA]←E911N[ALPHA]++/,F×M911P
[34]   F←CJR×IJ×IT4×(GM[1;;]×GP[2;;])-GM[2;;]×GP[1;;]
[35]   E1012N[ALPHA]←+/,F×M1012
[36]   →L1×⍳NMN≥ALPHA←ALPHA+1
[37]   E8N←RAW×E8N
[38]   E3N←RAW×E3N
[39]   HON←EN2BN+EN3BN+ENYUN
[40]   HVN←E8N+E911N+E1012N
[41]   HHN←E3N+E46N+E57N
[42]   ENTOTN←HON+HHN+HVN
[43]   ENSPN←(2×ENTOTN)+EN3BN-ENKEN
[44]   TENSPN←+/OCCN×ENSPN
[45]   ENKEN←E3N+E8N
[46]   ENEMCN←E46N+E911N
[47]   ENCURN←E57N+E1012N
[48]   TENKEN←+/OCCN×ENKEN
[49]   TENEMCN←+/,OCCN×ENEMCN
[50]   TENCURN←+/,OCCN×ENCURN
[51]   THON←+/,OCCN×HON
[52]   THHN←+/,OCCN×HHN
[53]   THVN←+/,OCCN×HVN
[54]   TENTOTN←+/,OCCN×ENTOTN
[55]   TEN2BN←+/,OCCN×EN2BN
[56]   TEN3BN←+/,OCCN×EN3BN
[57]   TE3N←+/,OCCN×E3N
[58]   TE46N←+/,OCCN×E46N
[59]   TE57N←+/,OCCN×E57N
[60]   TE8N←+/,OCCN×E8N
[61]   TE911N←+/,OCCN×E911N
[62]   TE1012N←+/,OCCN×E1012N
[63]   TENYUN←+/,OCCN×ENYUN
[64]   'LEAVING ENERN'
[65]   SPACE1
     ∇


     ∇ ENERP TP;MYU;M2B;M3B;M46;M57;M911S;M911P;M1012;F;GP;GM;MCE
[ 1]   SPACE1
[ 2]   'ENTERING ENERP'
[ 3]   ENCDP←ENYUP←ENCEP←EN2BP←EN3BP←E3P←E46P←E57P←NMP⍴0
[ 4]   E8P←E911P←E1012P←E3P
[ 5]   MCE←¯0.75×A[6]×PP*1÷3
```

```
[ 6]   MYU←0.5×(A[5]×UYP)+A[4]×UYN
[ 7]   M2B←0.5×(PP×A[1]-A[2])+A[1]×RN
[ 8]   M3B←0.5×A[3]×PN×PN+PP
[ 9]   M46←(2÷DZ×DZ)×KQ×TZP+KNQ×TZN
[10]   M57←(¯1÷DZ×DZ)×KQ×JZP+KNQ×JZN
[11]   M911S←(1÷DR×DR)×KQ×SP+KNQ×SN
[12]   M911P←KQ×PRP+KNQ×PRN
[13]   M1012←(¯1÷DR)×KQ×JRP+KNQ×JRN
[14]   ALPHA←1
[15] L1:G←FREAD(TP,ALPHA)
[16]   F←CP×+/[1]G×G
[17]   ENCDP[ALPHA]←0.5×+/,F×UCP
[18]   ENCEP[ALPHA]←+/,F×MCE
[19]   ENYUP[ALPHA]←+/,F×MYU
[20]   EN2BP[ALPHA]←+/,F×M2B
[21]   EN3BP[ALPHA]←+/,F×M3B
[22]   E911P[ALPHA]←+/,F×M911S
[23]   GP←0.5×(0 1↓F)+0 ¯1↓F
[24]   E46P[ALPHA]←+/,GP×M46
[25]   GP←0 0 1↓G
[26]   GM←0 0 ¯1↓G
[27]   F←CJZ×(GM[1;;]×GP[2;;])-GM[2;;]×GP[1;;]
[28]   E57P[ALPHA]←+/,F×M57
[29]   F←CTZ×+/[1]F×F←GM-GP
[30]   E3P[ALPHA]←B[1]×+/,F
[31]   F←(CS×MP[ALPHA]*2)×+/[1]G×G
[32]   E8P[ALPHA]←B[1]×+/,F×IS
[33]   GP←0 1 0↓G
[34]   GM←0 ¯1 0↓G
[35]   F←CTR×IT4×+/[1]F×F←(IT1×GM)-IT2×GP
[36]   E8P[ALPHA]←E8P[ALPHA]+B[1]×+/,F
[37]   E911P[ALPHA]←E911P[ALPHA]++/,F×M911P
[38]   F←CJR×IJ×IT4×(GM[1;;]×GP[2;;])-GM[2;;]×GP[1;;]
[39]   E1012P[ALPHA]←+/,F×M1012
[40]   →L1×⍳NMP≥ALPHA←ALPHA+1
[41]   E8P←RAW×E8P
[42]   E3P←RAW×E3P
[43]   HOP←EN2BP+EN3BP+ENYUP+ENCDP+ENCEP
[44]   HVP←E8P+E911P+E1012P
[45]   HHP←E3P+E46P+E57P
[46]   ENTOTP←HOP+HHP+HVP
[47]   ENSPP←(2×ENTOTP)+EN3BP-ENKEP
[48]   TENSPP←+/OCCP×ENSPP
[49]   ENKEP←E3P+E8P
[50]   ENEMCP←E46P+E911P
[51]   ENCURP←E57P+E1012P
[52]   TENKEP←+/OCCP×ENKEP
[53]   TENEMCP←+/,OCCP×ENEMCP
[54]   TENCURP←+/,OCCP×ENCURP
[55]   THOP←+/,OCCP×HOP
[56]   THHP←+/,OCCP×HHP
[57]   THVP←+/,OCCP×HVP
[58]   TENTOTP←+/,OCCP×ENTOTP
[59]   TENCD←+/,OCCP×ENCDP
```

```
[60]  TENCE←+/,OCCP×ENCEP
[61]  TEN2BP←+/,OCCP×EN2BP
[62]  TEN3BP←+/,OCCP×EN3BP
[63]  TE3P←+/,OCCP×E3P
[64]  TE46P←+/,OCCP×E46P
[65]  TE57P←+/,OCCP×E57P
[66]  TE8P←+/,OCCP×E8P
[67]  TE911P←+/,OCCP×E911P
[68]  TE1012P←+/,OCCP×E1012P
[69]  TENYUP←+/,OCCP×ENYUP
[70]  'LEAVING ENERP'
[71]  SPACE1
    ∇


    ∇ ENORDER I;P;NN;V;Q;ORDER;BACK;ORD;BA;STOP;OC;M;X
[ 1]  P←⎕PP
[ 2]  ⎕PP←8
[ 3]  EEN←ENSPN
[ 4]  DELENN←+/OCCN×(|(EEN*2)-EN*2)*0.5
[ 5]  ORDER←⍋EN
[ 6]  BACK←⍋ORDER
[ 7]  EN←EN[ORDER]
[ 8]  EEN←EEN[ORDER]
[ 9]  OCCN←OCCN[ORDER]
[10]  MN←MN[ORDER]
[11]  NN←+/OCCN
[12]  ORD←⍋EEN
[13]  BA←⍋ORD
[14]  M←MN[ORD]
[15]  V←NN<+\OC←2×1+M≠0
[16]  →L31×⍳NN=+/OC
[17]  STOP←¯1+1↑V/(⍳NMN)
[18]  OC←OC×1-V
[19]  →L25×⍳OC[STOP]=2×1+M[STOP]≠0
[20]  OC[STOP]←OC[STOP]+NN-+/OC
[21]  →L31
[22] L25:OC[STOP+1]←NN-+/OC
[23] L31:OC←OC[BA]
[24]  SPACE1
[25]  ' EN (OLD)     EN (NEW)     MN      OCCN(OLD)       OC'
[26]  ' '
[27]  X←'F10.2'⎕FRMT(⍉(5,⍴EN)⍴EN,EEN,MN,OCCN,OC)
[28]  X FWRITE(76,I)
[29]  X
[30]  ' WHICH METHOD DO YOU WANT TO USE TO CHANGE THE NEUTRON'
[31]  ' OCCUPATION NUMBERS:'
[32]  ' '
[33]  '     1- NO CHANGE'
[34]  '     2- MANUAL CHANGE'
[35]  '     3- AUTOMATIC FILLING OF LOWEST LEVELS'
[36]  ANSWER←⎕
[37]  →(L1,L2,L3)[ANSWER]
```

```
[38] L1:' NEW OCCUPATION NO. SAME AS OLD'
[39]  →L10
[40] L2:NN←+/OCCN
[41]  ' SUM OF OCCN BEFORE IS ';NN
[42]  ' HERE IS OCCN'
[43]  ' '
[44]  ⎕←(2,⍴OCCN)⍴(⍳⍴OCCN),OCCN
[45]  ' '
[46]  ' WHICH POSITION DO YOU WANT TO CHANGE'
[47]  V←⎕
[48]  ' ENTER NEW OCCUPATION QUANTUM NO.'
[49]  Q←⎕
[50]  →L2×⍳(+/Q)≠(+/OCCN[V])
[51]  OCCN[V]←Q
[52]  →L10
[53] L3:OCCN←OC
[54]  →L10
[55] L10:⎕PP←P
[56]  EN←EEN[BACK]
[57]  OCCN←OCCN[BACK]
[58]  MN←MN[BACK]
[59]  QNN[;7]←EN
[60]  QNN[;6]←OCCN
[61]  QNN[;8]←+\OCCN
[62]  QNN FWRITE(16,I)
[63]  '   DONE'
    ∇


    ∇  EPORDER I;P;NP;V;Q;ORDER;BACK;ORD;BA;STOP;OC;X
[ 1]  P←⎕PP
[ 2]  ⎕PP←8
[ 3]  EEP←ENSPP
[ 4]  DELENP←+/OCCP×(|(EEP⋆2)-EP⋆2)⋆0.5
[ 5]  ORDER←⍋EP
[ 6]  BACK←⍋ORDER
[ 7]  EP←EP[ORDER]
[ 8]  EEP←EEP[ORDER]
[ 9]  OCCP←OCCP[ORDER]
[10]  MP←MP[ORDER]
[11]  NP←+/OCCP
[12]  ORD←⍋EEP
[13]  BA←⍋ORD
[14]  M←MP[ORD]
[15]  V←NP≤+\OC←2×1+M≠0
[16]  →L31×⍳NP=+/OC
[17]  STOP←¯1+V/(⍳NMP)
[18]  OC←OC×1-V
[19]  →L25×⍳OC[STOP]=2×1+M[STOP]≠0
[20]  OC[STOP]←OC[STOP]+NP-+/OC
[21]  →L31
[22] L25:OC[STOP+1]←NP-+/OC
[23] L31:OC←OC[BA]
```

```
[24]  SPACE1
[25]  ' EP (OLD)    EP (NEW)     MP      OCCP(OLD)       OC'
[26]  ' '
[27]  X←'F10.2'⎕FRMT(⍉(5,⍴EP)⍴EP,EEP,MP,OCCP,OC)
[28]  X FWRITE(75,I)
[29]  X
[30]  ' WHICH METHOD DO YOU WANT TO USE TO CHANGE THE PROTON '
[31]  ' OCCUPATION NUMBERS:'
[32]  ' '
[33]  '     1- NO CHANGE'
[34]  '     2- MANUAL CHANGE'
[35]  '     3- AUTOMATIC FILLING OF LOWEST LEVELS'
[36]  ANSWER←⎕
[37]  →(L1,L2,L3)[ANSWER]
[38] L1:' NEW OCCUPATION NO. SAME AS OLD'
[39]  →L10
[40] L2:NP←+/OCCP
[41]  ' SUM OF OCCP BEFORE IS ';NP
[42]  ' HERE IS OCCP'
[43]  ' '
[44]  ⎕←(2,⍴OCCP)⍴(⍳⍴OCCP),OCCP
[45]  ' '
[46]  ' WHICH POSITION DO YOU WANT TO CHANGE'
[47]  V←⎕
[48]  ' ENTER NEW OCCUPATION QUANTUM NO.'
[49]  Q←⎕
[50]  →L2×⍳(+/Q)≠(+/OCCP[V])
[51]  OCCP[V]←Q
[52]  →L10
[53] L3:OCCP←OC
[54]  →L10
[55] L10:⎕PP←P
[56]  EP←EEP[BACK]
[57]  OCCP←OCCP[BACK]
[58]  MP←MP[BACK]
[59]  QNP[;7]←EP
[60]  QNP[;6]←OCCP
[61]  QNP[;8]←+\OCCP
[62]  QNP FWRITE(15,I)
[63]  '  DONE'
    ∇
```

```
    ∇ ERASEV;ZZI;ZZZ;ZZZZ;ZDUM
[1]  ' ENTER PASSWORD'
[2]  MAT←⍞
[3]  →0×⍳⍲/'ERASE VARIABLES '=16↑MAT
[4]  ZZZZ←⎕NL 2
[5]  ZZZ←(⍴ZZZZ)[1]
[6]  ZZI←1
[7]  ZDUM←⎕EX ZZZZ[ZZI;]
[8]  →7×⍳ZZZ≥ZZI←ZZI+1
    ∇
```

```
  ∇ ERLOCK;A
    A←⎕FX'FCREATE'
    A←⎕EX'FERASE'
    A←⎕EX'FNAMES'
    A←⎕EX'FNUMS'
    A←⎕EX'FREAD'
    A←⎕EX'FTIE'
    A←⎕EX'FUNTIE'
    A←⎕EX'FWRITE'
  ∇
```

```
  ∇ TNEW EVOLVEN TOLD;M;I;J;G14;G23;GOLD;ALPHA;DUM
    SPACE3
    '  ENTERING EVOLVEN FUNCTION'
    ' '
    IV←RV←(NZT,NR,NR)⍴0
    M←0
    RV[;1;1]←DON[1;]+0.5×HON[1;]
    RV[;1;2]←APN[1;1;]
    IV[;1;2]←APN[2;1;]
    I←2
   L1:RV[;I;I-1]←APN[1;(I-1);]
    IV[;I;I-1]←-APN[2;(I-1);]
    RV[;I;I]←DON[I;]+0.5×HON[I;]
    RV[;I;I+1]←APN[1;I;]
    IV[;I;I+1]←APN[2;I;]
    →L1×⍳NR>I←I+1
    RV[;NR;NR]←DON[NR;]+0.5×HON[NR;]
    RV[;NR;NR-1]←APN[1;(NR-1);]
    IV[;NR;NR-1]←-APN[2;(NR-1);]
    APN←DON←1
    →L1P5×⍳TTYPE=0
    DUM←RV
    RV←(-TS)×1 3 2⍉IV
    IV←TS×1 3 2⍉DUM
    DUM←1
    →L1P7
   L1P5:RV←TS×1 3 2⍉RV
    IV←TS×1 3 2⍉IV
   L1P7:ALPHA←1
   L2:G14←(2,NR,NZT)⍴0
    →L4×⍳MN[ALPHA]≠M
    GOLD←FREAD(TOLD,ALPHA)
    J←2
   L3:G14[1;;J]←(GOLD[1;;J]+.×RV[J;;])-GOLD[2;;J]+.×IV[J;;]
    G14[2;;J]←(GOLD[1;;J]+.×IV[J;;])+GOLD[2;;J]+.×RV[J;;]
    →L3×⍳NZT>J←J+1
    G14←GOLD-G14
    G14[;NR;]←0
    G14[;;(1,NZT)]←0
    G14 FWRITE(114,ALPHA)
    →L2×⍳NMN≥ALPHA←ALPHA+1
```

```
[ 41] L4:RV←1 3 2⍉RV
[ 42]  IV←1 3 2⍉IV
[ 43]  RV FWRITE(101,10+M)
[ 44]  IV FWRITE(102,10+M)
[ 45]  I←1
[ 46] L5:RV[;I;I]←1+RV[;I;I]
[ 47]  →L5×⍳NR≥I←I+1
[ 48] L8:J←2
[ 49] L9:G14←⌹RV[J;;]
[ 50]  RV[J;;]←⌹RV[J;;]+IV[J;;]+.×G14+.×IV[J;;]
[ 51]  IV[J;;]←-G14+.×IV[J;;]+.×RV[J;;]
[ 52]  →L9×⍳NZT>J←J+1
[ 53]  RV FWRITE(101,M)
[ 54]  IV FWRITE(102,M)
[ 55]  →L12×⍳ALPHA>NMN
[ 56]  RV←FREAD(101,10+M)
[ 57]  IV←FREAD(102,10+M)
[ 58]  M←M+1
[ 59]  I←1
[ 60]  →L10×⍳TTYPE=0
[ 61] L95:IV[;I;I]←IVE;I;I]+TS×(¯1+2×M)×CON1[I;]
[ 62]  →L95×⍳NR≥I←I+1
[ 63]  →L97
[ 64] L10:RV[;I;I]←RV[;I;I]+TS×(¯1+2×M)×CON1[I;]
[ 65]  →L10×⍳NR≥I←I+1
[ 66] L97:RV←1 3 2⍉RV
[ 67]  IV←1 3 2⍉IV
[ 68]  →L2
[ 69] L12:RV←IV←1
[ 70]  IH←RH←(NR,NZT,NZT)⍴0
[ 71]  RH[;1;1]←BON[;1]+0.5×HON[;1]
[ 72]  RH[;1;2]←BPN[1;;1]
[ 73]  IH[;1;2]←-BPN[2;;1]
[ 74]  I←2
[ 75] L13:RH[;I;I-1]←BPN[1;;I-1]
[ 76]  IH[;I;I-1]←BPN[2;;I-1]
[ 77]  RH[;I;I]←BON[;I]+0.5×HON[;I]
[ 78]  RH[;I;I+1]←BPN[1;;I]
[ 79]  IH[;I;I+1]←-BPN[2;;I]
[ 80]  →L13×⍳NZT>I←I+1
[ 81]  RH[;NZT;NZT]←BON[;NZT]+0.5×HON[;NZT]
[ 82]  RH[;NZT;NZT-1]←BPN[1;;NZT-1]
[ 83]  IH[;NZT;NZT-1]←BPN[2;;NZT-1]
[ 84]  BPN←BON←HON←1
[ 85]  →L14×⍳TTYPE=0
[ 86]  DUM←RH
[ 87]  RH←(-TS)×IH
[ 88]  IH←TS×DUM
[ 89]  DUM←1
[ 90]  →L15
[ 91] L14:RH←TS×RH
[ 92]  IH←TS×IH
[ 93] L15:I←1
[ 94] L16:RH[;I;I]←1+RH[;I;I]
```

```
[ 95]  →L16×⍳NZT≥I←I+1
[ 96]  I←1
[ 97] L18:G14←⌹RH[I;;]
[ 98]  RH[I;;]←⌹RH[I;;]+IH[I;;]+.×G14+.×IH[I;;]
[ 99]  IH[I;;]←-G14+.×IH[I;;]+.×RH[I;;]
[100]  →L18×⍳NR>I←I+1
[101]  G23←(2,NR,NZT)⍴0
[102]  ALPHA←1
[103] L20:G14←FREAD(114,ALPHA)
[104]  I←1
[105] L21:G23[1;I;]←(G14[1;I;]+.×RH[I;;])-G14[2;I;]+.×IH[I;;]
[106]  G23[2;I;]←(G14[2;I;]+.×RH[I;;])+G14[1;I;]+.×IH[I;;]
[107]  →L21×⍳NR>I←I+1
[108]  G23←(2×G23)-G14
[109]  G23[;NR;]←0
[110]  G23[;;(1,NZT)]←0
[111]  G23 FWRITE(123,ALPHA)
[112]  →L20×⍳NMN≥ALPHA←ALPHA+1
[113]  RH←IH←1
[114]  ALPHA←1
[115]  M←¯1
[116]  G14←(2,NR,NZT)⍴0
[117] L22:M←M+1
[118]  →L25×⍳M>15
[119]  →L22×⍳MN[ALPHA]≠M
[120]  RV←FREAD(101,M)
[121]  IV←FREAD(102,M)
[122] L23:→L22×⍳MN[ALPHA]≠M
[123]  RV←1 3 2⍉RV
[124]  IV←1 3 2⍉IV
[125]  G23←FREAD(123,ALPHA)
[126]  J←2
[127] L24:G14[1;;J]←(G23[1;;J]+.×RV[J;;])-G23[2;;J]+.×IV[J;;]
[128]  G14[2;;J]←(G23[2;;J]+.×RV[J;;])+G23[1;;J]+.×IV[J;;]
[129]  →L24×⍳NZT>J←J+1
[130]  G14[;;(1,NZT)]←0
[131]  G14[;NR;]←0
[132]  G14 FWRITE(TNEW,ALPHA)
[133]  →L23×⍳NMN≥ALPHA←ALPHA+1
[134]  IV←RV←1
[135] ('TIME EVOLUTION DONE FOR NEUTRONS'
[136]  SPACE1
[137]  ' LEAVING EVOLVEN FUNCTION'
[138]  SPACE3
[139]  →0
[140] L25:' M IS ';M;' ,  MUST STOP'
[141]  I←⎕
    ∇


    ∇  TNEW EVOLVEP TOLD;M;I;J;G14;G23;GOLD;ALPHA;DUM
[  1]  SPACE3
[  2]  '  ENTERING EVOLVEP FUNCTION'
```

```
[  3]
[  4]  IV←RV←(NZT,NR,NR)⍴0
[  5]  M←0
[  6]  RV[;1;1]←DOP[1;]+0.5×HOP[1;]
[  7]  RV[;1;2]←APP[1;1;]
[  8]  IV[;1;2]←APP[2;1;]
[  9]  I←2
[ 10] L1:RV[;I;I-1]←APP[1;(I-1);]
[ 11]  IV[;I;I-1]←-APP[2;(I-1);]
[ 12]  RV[;I;1]←DOP[I;]+0.5×HOP[I;]
[ 13]  RV[;I;I+1]←APP[1;I;]
[ 14]  IV[;I;I+1]←APP[2;I;]
[ 15]  →L1×⍳NR>I←I+1
[ 16]  RV[;NR;NR]←DOP[NR;]+0.5×HOP[NR;]
[ 17]  RV[;NR;NR-1]←APP[1;(NR-1);]
[ 18]  IV[;NR;NR-1]←-APP[2;(NR-1);]
[ 19]  APP←DOP←1
[ 20]  →L1P5×⍳TTYPE=0
[ 21]  DUM←RV
[ 22]  RV←(-TS)×1 3 2⍉IV
[ 23]  IV←TS×1 3 2⍉DUM
[ 24]  DUM←1
[ 25]  →L1P7
[ 26] L1P5:RV←TS×1 3 2⍉RV
[ 27]  IV←TS×1 3 2⍉IV
[ 28] L1P7:ALPHA←1
[ 29] L2:G14←(2,NR,NZT)⍴0
[ 30]  →L4×⍳MP[ALPHA]≠M
[ 31]  GOLD←FREAD(TOLD,ALPHA)
[ 32]  J←2
[ 33] L3:G14[1;;J]←(GOLD[1;;J]+.×RV[J;;])-GOLD[2;;J]+.×IV[J;;]
[ 34]  G14[2;;J]←(GOLD[1;;J]+.×IV[J;;])+GOLD[2;;J]+.×RV[J;;]
[ 35]  →L3×⍳NZT>J←J+1
[ 36]  G14←GOLD-G14
[ 37]  G14[;NR;]←0
[ 38]  G14[;;(1,NZT)]←0
[ 39]  G14 FWRITE(114,ALPHA)
[ 40]  →L2×⍳NMP≥ALPHA←ALPHA+1
[ 41] L4:RV←1 3 2⍉RV
[ 42]  IV←1 3 2⍉IV
[ 43]  RV FWRITE(101,10+M)
[ 44]  IV FWRITE(102,10+M)
[ 45]  I←1
[ 46] L5:RV[;I;I]←1+RV[;I;I]
[ 47]  →L5×⍳NR≥I←I+1
[ 48] L8:J←2
[ 49] L9:G14←⌹RV[J;;]
[ 50]  RV[J;;]←⌹RV[J;;]+IV[J;;]+.×G14+.×IV[J;;]
[ 51]  IV[J;;]←-G14+.×IV[J;;]+.×RV[J;;]
[ 52]  →L9×⍳NZT>J←J+1
[ 53]  RV FWRITE(101,M)
[ 54]  IV FWRITE(102,M)
[ 55]  →L12×⍳ALPHA>NMP
[ 56]  RV←FREAD(101,10+M)
```

```
[ 57]  IV←FREAD(102,10+M)
[ 58]  M←M+1
[ 59]  I←1
[ 60]  →L10×⍳TTYPE=0
[ 61] L95:IV[;I;I]←IV[;I;I]+TS×(¯1+2×M)×COP1[I;]
[ 62]  )L95×⍳NR≥I←I+1
[ 63]  →L97
[ 64] L10:RV[;I;I]←RV[;I;I]+TS×(¯1+2×M)×COP1[I;]
[ 65]  →L10×⍳NR≥I←I+1
[ 66] L97:RV←1 3 2⍉RV
[ 67]  IV←1 3 2⍉IV
[ 68]  →L2
[ 69] L12:RV←IV←1
[ 70]  IH←RH←(NR,NZT,NZT)⍴0
[ 71]  RH[;1;1]←BOF[;1]+0.5×HOF[;1]
[ 72]  RH[;1;2]←BPF[1;;1]
[ 73]  IH[;1;2]←-BPF[2;;1]
[ 74]  I←2
[ 75] L13:RH[;I;I-1]←BPF[1;;I-1]
[ 76]  IH[;I;I-1]←BPF[2;;I-1]
[ 77]  RH[;I;I]←BOF[;I]+0.5×HOF[;I]
[ 78]  RH[;I;I+1]←BPF[1;;I]
[ 79]  IH[;I;I+1]←-BPF[2;;I]
[ 80]  →L13×⍳NZT>I←I+1
[ 81]  RH[;NZT;NZT]←BOF[;NZT]+0.5×HOF[;NZT]
[ 82]  RH[;NZT;NZT-1]←BPF[1;;NZT-1]
[ 83]  IH[;NZT;NZT-1]←BPF[2;;NZT-1]
[ 84]  BPF←BOF←HOF←1
[ 85]  →L14×⍳TTYPE=0
[ 86]  DUM←RH
[ 87]  RH←(-TS)×IH
[ 88]  IH←TS×DUM
[ 89]  DUM←1
[ 90]  →L15
[ 91] L14:RH←TS×RH
[ 92]  IH←TS×IH
[ 93] L15:I←1
[ 94] L16:RH[;I;I]←1+RH[;I;I]
[ 95]  →L16×⍳NZT≥I←I+1
[ 96]  I←1
[ 97] L18:G14←⌹RH[I;;]
[ 98]  RH[I;;]←⌹RH[I;;]+IH[I;;]+.×G14+.×IH[I;;]
[ 99]  IH[I;;]←-G14+.×IH[I;;]+.×RH[I;;]
[100]  →L18×⍳NR>I←I+1
[101]  G23←(2,NR,NZT)⍴0
[102]  ALPHA←1
[103] L20:G14←FREAD(114,ALPHA)
[104]  I←1
[105] L21:G23[1;I;]←(G14[1;I;]+.×RH[I;;])-G14[2;I;]+.×IH[I;;]
[106]  G23[2;I;]←(G14[2;I;]+.×RH[I;;])+G14[1;I;]+.×IH[I;;]
[107]  →L21×⍳NR>I←I+1
[108]  G23←(2×G23)-G14
[109]  G23[;NR;]←0
[110]  G23[;;(1,NZT)]←0
```

```
[111]  G23 FWRITE(123,ALPHA)
[112]  →L20×⍳NMP≥ALPHA←ALPHA+1
[113]  RH←IH←1
[114]  ALPHA←[illegible]
[115]  M←¯1
[116]  G14←(2,NR,NZT)⍴0
[117] L22:M←M+1
[118]  →L25×⍳M>15
[119]  →L32×⍳MP[ALPHA]≠M
[120]  RV←FREAD(101,M)
[121]  IV←FREAD(102,M)
[122] L23:→L22×⍳MP[ALPHA]≠M
[123]  RV←1 3 2⍉RV
[124]  IV←1 3 2⍉IV
[125]  G23←FREAD(123,ALPHA)
[126]  J←2
[127] L24:G14[1;;J]←(G23[1;;J]+.×RV[J;;])-G23[2;;J]+.×IV[J;;]
[128]  G14[2;;J]←(G23[2;;J]+.×RV[J;;])+G23[1;;J]+.×IV[J;;]
[129]  →L24×⍳NZT>J←J+1
[130]  G14[;;(1,NZT)]←0
[131]  G14[;NR;]←0
[132]  G14 FWRITE(TNEW,ALPHA)
[133]  →L23×⍳NMP≥ALPHA←ALPHA+1
[134]  IV←RV←1
[135]  'TIME EVOLUTION DONE FOR PROTONS'
[136]  SPACE1
[137]  ' LEAVING EVOLVEP FUNCTION'
[138]  SPACE3
[139]  →0
[140] L25:' M IS ';M;' ,  MUST STOP'
[141]  I←⎕
    ∇


    ∇ NAME FSAVE TIENUM;L;T;V;U
[ 1]  NAME←NAME[(NAME≠' ')/⍳⍴NAME]
[ 2]  L←⍴NAME
[ 3]  T←⍴,FNUMS
[ 4]  →L1×⍳T=0
[ 5]  T←⍴V←(TIENUM=,FNUMS)/(⍳T)
[ 6]  →L2×⍳T=0
[ 7]  T←FNAMES
[ 8]  →L3×⍳L≠+/NAME=U←1↓,T[V;⍳L+1]
[ 9]  FUNTIE TIENUM
[10]  NAME FTIE TIENUM
[11]  NAME,'  SAVED  '
[12]  →0
[13] L1:'  THERE ARE NO FILES TIED'
[14]  →0
[15] L2:'  THERE ARE NO FILES TIED TO THIS NUMBER'
[16]  →0
[17] L3:'  NO MATCH BETWEEN FILE NAME GIVEN AND TIE NUMBER'
    ∇
```

```
    ∇  Z←GOIF A;B
[1]    B←0
[2]    Z←⍳A=1↑[illegible]B
    ∇
```

```
     ∇   GM GRAM TIE;GREF;GSTOP;ALPHA;UJ;X;SUM;U;ESUM;N1;N2
[ 1]     SET←(GM=M)/(⍳STOP)
[ 2]     GE←E[SET]
[ 3]     GREF←REF[SET;]
[ 4]     GSTOP←⍴SET
[ 5]     ALPHA←1
[ 6]   L1:X←FREAD GREF[ALPHA;]
[ 7]     SUM←0
[ 8]     ESUM←0
[ 9]     →L3×⍳ALPHA=1
[10]     I←1
[11]   L2:UJ←FREAD GREF[I;]
[12]     G[1;;]←(X[1;;]×UJ[1;;])+X[2;;]×UJ[2;;]
[13]     G[2;;]←(X[1;;]×UJ[2;;])-X[2;;]×UJ[1;;]
[14]     N1←V×+/,G[1;;]
[15]     N2←V×+/,G[2;;]
[16]     UJ[1;;]←UJ[1;;]×N1
[17]     UJ[2;;]←UJ[2;;]×N2
[18]     SUM←SUM+UJ
[19]     ESUM←ESUM+N1×GE[I]
[20]     →L2×⍳ALPHA≥I←I+1
[21]   L3:U←X-SUM
[22]     GE[ALPHA]←GE[ALPHA]-ESUM
[23]     U[;;1]←U[;;NZT]←0
[24]     U[;NR;]←0
[25]     U←U×WFNORM U
[26]     U FWRITE GREF[ALPHA;]
[27]     →L1×⍳GSTOP≥ALPHA←ALPHA+1
     ∇
```

```
     ∇   NTIE GRAMSCH PTIE;V;STOP;MSTOP;M;GM;REF;E;GE
[ 1]     SPACE1
[ 2]     'ENTERING GRAMSCH'
[ 3]     V←DR×DR×DZ×○2
[ 4]     STOP←NMP
[ 5]     REF←⍉(2,NMP)⍴(NMP⍴PTIE),⍳NMP
[ 6]     M←MP
[ 7]     E←EP
[ 8]     MSTOP←⌈/M
[ 9]     G←FREAD(PTIE,1)
[10]     GM←0
[11]   L1:GM GRAM PTIE
[12]     EP[SET]←GE
[13]     →L1×⍳MSTOP≥GM←GM+1
[14]     STOP←NMN
```

```
[15]  M←MN
[16]  E←EN
[17]  MSTOP←⌈/M
[18]  REF←⍉(2,NMN)⍴(NMN⍴NTIE),⍳NMN
[19]  GM←0
[20] L2:GM GRAM NTIE
[21]  →L2×⍳MSTOP≥GM←GM+1
[22]  SPACE1
[23]  'LEAVING GRAMSCH'
[24]  SPACE1
    ∇
```

```
    ∇ HALFDEN
[ 1]  PP←0.5×PP+FREAD 400 1
[ 2]  PN←0.5×PN+FREAD 400 2
[ 3]  PRP←0.5×PRP+FREAD 400 3
[ 4]  PRN←0.5×PRN+FREAD 400 4
[ 5]  PZP←0.5×PZP+FREAD 400 5
[ 6]  PZN←0.5×PZN+FREAD 400 6
[ 7]  JRP←0.5×JRP+FREAD 400 7
[ 8]  JRN←0.5×JRN+FREAD 400 8
[ 9]  JZP←0.5×JZP+FREAD 400 9
[10]  JZN←0.5×JZN+FREAD 400 10
[11]  TRP←0.5×TRP+FREAD 400 11
[12]  TRN←0.5×TRN+FREAD 400 12
[13]  TZP←0.5×TZP+FREAD 400 13
[14]  TZN←0.5×TZN+FREAD 400 14
[15]  SP←0.5×SP+FREAD 400 15
[16]  SN←0.5×SN+FREAD 400 16
    ∇
```

```
     ∇ INITIAL;L;LL;I;P;J;MAX;WF;QN;RMAT;ZMAT;ALPHA;GAMMA;STOP
[  1]  SPACE3
[  2]  '  ENTERING INITIAL FUNCTION'
[  3]  ' '
[  4]  '  INPUT NO. OF NEUTRONS'
[  5]  NN←⎕
[  6]  '  INPUT NO. OF PROTONS'
[  7]  NP←⎕
[  8]  'ENTER MAX. NO. OF SHELLS'
[  9]  'NOTE THAT THE LEVELS WITH M≠0 HAVE DEGENERACY 4 AND THOSE'
[ 10]  'FOR M=0 HAVE DEGENARACY 2 (I.E. SPIN UP AND SPIN DOWN)'
[ 11]  ⎕←2 10⍴I,(I+1)×(I+2)×(3+I←⍳10)÷3
[ 12]  L←⎕
[ 13]  LL←((L+2)×(L+3)×(5+2×L)÷24)-(L(L+3)÷2)÷4
[ 14]  QUANTO L
[ 15]  '  INPUT DEFORMATION PARAMETER DELTA'
[ 16]  DEL←⎕
[ 17]  HWOO←41.43×(NP+NN)*(÷¯3)
[ 18]  HWO←HWOO×(1-((4÷3)×DEL*2)+(16÷27)×DEL*3)*(÷¯6)
```

```
[ 19]  HWT←HWO×(1+2×DEL÷3)*0.5
[ 20]  HWZ←HWO×(1-4×DEL÷3)*0.5
[ 21]  ALPHA←0.0241×HWT
[ 22]  GAMMA←0.0241×HWZ
[ 23]  I←NN,NP,DEL,HWOO,HWO,HWT,HWZ,ALPHA,GAMMA
[ 24]  I FWRITE 11 29
[ 25]  QN[;7]←(HWZ×(QN[;4]+0.5))+HWT×(1+QN[;5]+2×QN[;3])
[ 26]  I←QN[;1]
[ 27]  QN←QN[(⍋QN[;7]);]
[ 28]  QN[;1]←I
[ 29]  '  DO YOU WANT A DISPLAY OF THE SET OF QUANTUM '
[ 30]  '  NUMBERS,  IN ORDER OF ENERGY'
[ 31]  →L2×GOIF'N'
[ 32]  P←⎕PP
[ 33]  ⎕PP←5
[ 34]  '  UP TO WHAT LEVEL DO YOU WANT TO SEE'
[ 35]  QN[;8]←+\QN[;6]
[ 36]  (2,LL)⍴QN[;1],QN[;8]
[ 37]  I←⎕
[ 38]  ' '
[ 39]  DES←'S N NR NZ M NAL E   COUNT'
[ 40]  DES
[ 41]  ⎕←QN[(⍳I);]
[ 42] L2:'  ENTER NO. OF LAST PROTON LEVEL DESIRED (ENTER NO.'
[ 43]  '  FROM COLUMN 1)'
[ 44]  NMP←⎕
[ 45]  QNP←(NMP,8)↑QN
[ 46]  '  ENTER NO. OF LAST NEUTRON LEVEL DESIRED (ENTER NO.'
[ 47]  '  FROM COLUMN 1)'
[ 48]  NMN←⎕
[ 49]  QNN←(NMN,8)↑QN
[ 50]  ' IS THE FILLING APPROXIMATION TO BE USED'
[ 51]  →L3×GOIF'N'
[ 52]  '  ENTER WHICH OCCUPATION NO. (COL 6) OF THE PROTON LEVELS'
[ 53]  '  ARE TO BE CHANGED (ENTER NO. FROM COLUMN 1)'
[ 54]  I←⎕
[ 55]  '  ENTER NEW OCCUPATION NUMBERS IN THE SAME ORDER AS ABOVE'
[ 56]  J←⎕
[ 57]  QNP[I;6]←J
[ 58]  '  ENTER WHICH OCCUPATION NO. (COLUMN 6) OF THE NEUTRON'
[ 59]  '  LEVELS ARE TO BE CHANGED (ENTER NO. FROM COLUMN 1)'
[ 60]  I←⎕
[ 61]  '  ENTER NEW OCCUPATION NUMBERS IN THE SAME ORDER AS ABOVE'
[ 62]  J←⎕
[ 63]  QNN[I;6]←J
[ 64] L3:→L4×⍳(NN=+/QNN[;6])∧NP=+/QNP[;6]
[ 65]  ' SUM OF OCCUPATION NO. DOES NOT REPRESENT NUMBER '
[ 66]  ' OF NUCLEONS'
[ 67]  →L2
[ 68] L4:QNN[;8]←+\QNN[;6]
[ 69]  QNP[;8]←+\QNP[;6]
[ 70]  '  DO YOU WANT A DISPLAY OF THE FINAL QUANTUM NO.'
[ 71]  →L5×GOIF'N'
[ 72]  ⎕←DES,' (PROTON LEVELS)'
```

```
[ 73]  ⎕←QNP
[ 74]  ' '
[ 75]  ⎕←DES,'   (NEUTRON LEVELS)'
[ 76]  ⎕←QNN
[ 77]  ' ANY MAJOR CORRECTIONS'
[ 78]  →L2×GOIF'Y'
[ 79] L5:I←QNP[;1]
[ 80]  QNP←QNP[(⍋QNP[;5]);]
[ 81]  QNP[;8]←+\QNP[;6]
[ 82]  QNP[;1]←I
[ 83]  I←QNN[;1]
[ 84]  QNN←QNN[(⍋QNN[;5]);]
[ 85]  QNN[;8]←+\QNN[;6]
[ 86]  QNN[;1]←I
[ 87]  '   HERE IS A DISPLAY OF THE FINAL QUANTUM NO.'
[ 88]  ' IN INCREASING ORDER OF AZIMUTHAL QUANTUM NO. M'
[ 89]  ⎕←DES,' (PROTON LEVELS)'
[ 90]  ⎕←QNP
[ 91]  ' '
[ 92]  ⎕←DES,' (NEUTRON LEVELS)'
[ 93]  ⎕←QNN
[ 94]  MAX←⌈/(QNN[;3 4 5]),QNP[;3 4 5]
[ 95]  ZED MAX[2]
[ 96]  (MAX[3])RADIAL MAX[1]
[ 97]  I←NZ,NZT,DZ,NR,DR,NMN,NMP
[ 98]  I FWRITE 11 30
[ 99]  '   ENTER NO. OF LAST ROW IN WHICH NEUTRON QUANTUM NO.'
[100]  ' AND PROTON QUANTUM NO. ARE IDENTICAL'
[101]  STOP←⎕
[102]  STOP←STOP⌊NMN⌊NMP
[103]  '   ENTER PERMANENT FILE NAME FOR PROTON WAVEFNC'
[104]  F1←⍞
[105]  '   ENTER PERMANENT FILE NAME FOR NEUTRON WAVEFNC'
[106]  F2←⍞
[107]  '   ENTER FILE TIE NUMBER FOR FILE   ',F1
[108]  T1←⎕
[109]  '   ENTER FILE TIE NUMBER FOR FILE   ',F2
[110]  T2←⎕
[111]  I←F1;SPACE1;T1;SPACE1;F2;SPACE1;T2
[112]  I FWRITE 11 31
[113]  ' DO WE NEED TO CREATE THESE FILES'
[114]  →L51×GOIF'N'
[115]  F1 FCREATE T1
[116]  F2 FCREATE T2
[117]  →L59
[118] L51:' IS THE PROTON FILE ';F1;' TIED'
[119]  →L52×GOIF'Y'
[120]  F1 FTIE T1
[121] L52:' IS THE NEUTRON FILE ';F2;' TIED'
[122]  →L59×GOIF'Y'
[123]  F2 FTIE T2
[124] L59:OCCP←QNP[;6]
[125]  OCCN←QNN[;6]
[126]  MP←QNP[;5]
```

```
[127]  MN←QNN[;5]
[128]  EP←QNP[;7]
[129]  EN←QNN[;7]
[130]  I←1
[131]  WF←(2,NR,NZT)⍴0
[132]  NMP;' DIFFERENT PROTON  LEVELS USED FOR THE ';NP;' PROTONS'
[133]  NMN;' DIFFERENT NEUTRON LEVELS USED FOR THE ';NN;' NEUTRONS'
[134] L6:WFN QNP[I;3 4 5]
[135]  WF FWRITE(T1,I)
[136]  WF FWRITE(T2,I)
[137]  1 DENHO WF
[138]  →L6×⍳STOP≥I←I+1
[139]  ' THE ';STOP;' COMMON PROTON AND NEUTRON LEVELS ARE DONE'
[140]  J←I←I-1
[141] L7:→L8×⍳NMP<I←I+1
[142]  WFN QNP[I;3 4 5]
[143]  WF FWRITE(T1,I)
[144]  2 DENHO WF
[145]  →L7
[146] L8:I←J
[147]  ' THE ';NMP;' PROTON LEVELS ARE DONE'
[148] L9:→L10×⍳NMN<I←I+1
[149]  WFN QNN[I;3 4 5]
[150]  WF FWRITE(T2,I)
[151]  3 DENHO WF
[152]  →L9
[153] L10:SDENHO
[154]  ' THE ';NMN;' NEUTRON LEVELS ARE DONE'
[155]  TDENS
[156]  T2 GRAMSCH T1
[157]  F1 FSAVE T1
[158]  F2 FSAVE T2
[159]  QNN FWRITE 16 0
[160]  QNP FWRITE 15 0
[161]  ' LEAVING INITIAL FUNCTION'
[162]  SPACE3
     ∇


     ∇ LIST;MAT;F;AT;FUNCS;A;B;C;STOP;LM;TM;BM;LP;I;R
[ 1]  FUNCS←⎕NL 3
[ 2]  ERLOCK
[ 3]  LM←1
[ 4]  TM←1
[ 5]  BM←1
[ 6]  LP←11
[ 7]  'ENTER PAGE NO, WE START AT'
[ 8]  PAGENO←⎕
[ 9]  LEFTMAR←⌈10×LM
[10]  LTM←¯4+⌈6×TM
[11]  LBM←⌈6×BM
[12]  SLBM←(LBM,1)⍴' '
[13]  LLP←⌈6×LF
```

```
[14]   MAXLIN←LLP-LTM+LBM+4
[15]   A←3 1⍴' '
[16]   B←(68⍴' '),'A-'
[17]   C←(LTM,1)⍴' '
[18]   MAT←⎕NL 3
[19]   STOP←(⍴MAT)[1]
[20]   FNSNO←1
[21]   FREELIN←MAXLIN
[22]   'ADJUST PAPER'
[23]   I←⍞
[24]   A
[25]   B;PAGENO
[26]   C
[27]  L1:F←⎕CR MAT[FNSNO;]
[28]   FLINES←(⍴F)[1]
[29]   AT←⍕((FLINES,1)⍴¯1+⍳FLINES)
[30]   ML←(FLINES,LEFTMAR)⍴' '
[31]   F←ML,'[',AT,']',' ',F
[32]   D←LEFTMAR+2+(⍴AT)[2]
[33]   T←((D-1)⍴' '),'∇'
[34]   F[1;(⍳D)]←T
[35]   SHOWED←0
[36]  L3:SHOW←FREELIN⌊FLINES
[37]   R←SHOWED+⍳SHOW
[38]   F[R;]
[39]   SHOWED←SHOWED+SHOW
[40]   →L5×⍳FLINES≤FREELIN
[41]   FLINES←FLINES-FREELIN
[42]   FREELIN←MAXLIN
[43]   PAGENO←PAGENO+1
[44]   SLBM
[45]   A
[46]   B;PAGENO
[47]   C
[48]   →L3
[49]  L5:T
[50]   FREELIN←FREELIN-FLINES+1
[51]   →L20×⍳STOP<FNSNO←FNSNO+1
[52]   →L10×⍳FREELIN≤5
[53]   A
[54]   FREELIN←FREELIN-3
[55]   →L1
[56]  L10:⎕←((FREELIN+LBM),1)⍴' '
[57]   FREELIN←MAXLIN
[58]   PAGENO←PAGENO+1
[59]   A
[60]   B;PAGENO
[61]   C
[62]   →L1
[63]  L20:((FREELIN+LBM),1)⍴' '
[64]   A
[65]   'THE FUNCTIONS ARE LISTED'
     ∇
```

```
    ∇ LISTFNS;W;LM;TM;LTM;BM;LBM;LP;NLINES;LEFTMAR;MAXLIN;MAT
[ 1]  'ARE THE LOCKED FNS  ERASED?'
[ 2]  →0×GOIF'N'
[ 3]  'INPUT PRINTING WIDTH (10 CHARACTERS PER INCH)'
[ 4]  W←⎕
[ 5]  'ENTER SIZE OF LEFT HAND MARGIN'
[ 6]  LM←⎕
[ 7]  'ENTER SIZE OF TOP MARGIN'
[ 8]  TM←⎕
[ 9]  LTM←⌈6×TM
[10]  'ENTER SIZE OF BOTTOM MARGIN'
[11]  BM←⎕
[12]  LBM←⌈6×BM
[13]  'ENTER LENGTH OF PAPER'
[14]  LP←⎕
[15]  NLINES←⌈6×LP-BM+TM
[16]  LEFTMAR←⌈10×LM
[17]  MAXLIN←⌈6×LP
[18]  SKIP←LBM+LTM
[19]  SLBM←(LBM,1)⍴' '
[20]  SLTM←(LTM,1)⍴' '
[21]  MAT←⎕NL 3
[22]  STOP←(⍴MAT)[1]
[23]  I←1
[24]  'ADJUST PAPER AND PRESS RETURN'
[25]  A←⍞
[26] L1:NLINES LOOK1 MAT[I;]
[27]  I←I+1
[28]  →L1×I≤STOP
    ∇


    ∇ MAINORM;N;A
[ 1]  SPACE3
[ 2]  ' DO WE LOOK AT THE NORM OF THE DENSITIES'
[ 3]  →0×GOIF'N'
[ 4]  N←' PP   '
[ 5]  1 NORMAIN PP
[ 6]  N←' PN   '
[ 7]  2 NORMAIN PN
[ 8]  →L1×⍳TTYPE=0
[ 9]  N←' JRP '
[10]  7 NORMAIN JRP
[11]  N←' JRN '
[12]  8 NORMAIN JRN
[13]  N←' JZP '
[14]  9 NORMAIN JZP
[15]  N←' JZN '
[16]  10 NORMAIN JZN
[17] L1:N←' TRP '
[18]  11 NORMAIN TRP
[19]  N←' TRN '
[20]  12 NORMAIN TRN
```

```
[21]  N←' TZP '
[22]  13 NORMAIN TZP
[23]  N←' TZN '
[24]  14 NORMAIN TZN
[25]  N←' SP  '
[26]  15 NORMAIN SP
[27]  N←' SN  '
[28]  16 NORMAIN SN
[29]  SPACE2
    ∇


    ∇  MPFIXL;I;Q
[ 1]  'OLD LAMBDA 2,  LAMBDA 3,  LAMBDA 4:'
[ 2]  ⎕←LAMBD2,LAMBD3,LAMBD4
[ 3]  'ENTER NEW VALUES FOR THE LAMBDAS'
[ 4]  I←⎕
[ 5]  I←3⍴,I
[ 6]  LAMBD2H←I[1]
[ 7]  LAMBD3H←I[2]
[ 8]  LAMBD4H←I[3]
[ 9]  'OLD Q2, Q3, Q4'
[10]  ⎕←Q2,Q3,Q4
[11]  'ENTER NEW VALUES FOR THE Q''S'
[12]  Q←⎕
[13]  Q←3⍴,Q
[14]  Q2←Q[1]
[15]  Q3←Q[2]
[16]  Q4←Q[3]
    ∇


    ∇  MPMEAS;VI;A;R2Y20;R2Y30;R2Y40;Z;P;B;C;T;L;S
[ 1]  →L1×ιITIME≠0
[ 2]  Q20←Q30←Q40←LAMBD2←LAMBD3←LAMBD4←ZZ0←Q2←Q3←Q4←0
[ 3]  LAMBD2H←LAMBD3H←LAMBD4H←RSEP←Q2H←Q3H←Q4H←0
[ 4]  RMST←RMSP←RMSN←0
[ 5] L1:MPTERMS
[ 6]  Z←DZ×NZT-1
[ 7]  P←⎕PP
[ 8]  ⎕PP←5
[ 9]  SPACE2
[10]  B←FREAD 11 32
[11]  C←AH,AH,RSEP,RSEPH,ZZ0,ZZ0H,LAMBD2,LAMBD2H,Q2,Q2H
[12]  C←C,Q20,Q20H,LAMBD3
[13]  C←C,LAMBD3H,Q3,Q3H,Q30,Q30H,LAMBD4,LAMBD4H
[14]  C←C,Q4,Q4H,Q40,Q40H,RMST,RMSTH
[15]  C←15 2⍴C,RMSP,RMSPH,RMSN,RMSNH
[16]  C←'F10.3'⎕FRMT C
[17]  Z←,'F4.1'⎕FRMT Z
[18]  B←B,C
[19]  T←55↑(41⍴' '),'OLD        NEW'
```

```
[20]  S←55ρ' '
[21]  L←(4,55)ρS,T,55↑'RANGE OF Z ';(24ρ'.'),'    0-',Z,'     0-',Z
[22]  B←L,B
[23]  ⎕←B
[24]  B FWRITE(100,ITIME)
[25]  WAIT
[26]  LAMBD2←LAMBD2H
[27]  LAMBD3←LAMBD3H
[28]  LAMBD4←LAMBD4H
[29]  Q20←Q20H
[30]  Q30←Q30H
[31]  Q40←Q40H
[32]  ZZO←ZZOH
[33]  Q2←Q2H
[34]  Q3←Q3H
[35]  Q4←Q4H
[36]  RSEP←RSEPH
[37]  RMST←RMSTH
[38]  RMSP←RMSPH
[39]  RMSN←RMSNH
[40]  ⎕PP←P
    ∇


    ∇ MPTERMS;Z;ZP;R;RP2;COS1;COS2;RP3;RP4;R2Y20;R3Y30;R4Y40
[ 1]  VI←(DR×DZ×○2)×R←DR×⍉(NZT,NR)ρ¯0.5+⍳NR
[ 2]  AH←+/,VI×PP+PN
[ 3]  Z←DZ×(NR,NZT)ρ¯1+⍳NZT
[ 4]  ZZOH←(+/,Z×VI×PP+PN)÷AH
[ 5]  RSEPH←(÷AH)×+/,VI×(PP+PN)×|Z-ZZOH
[ 6]  ZP←Z-ZZOH
[ 7]  RP2←(ZP*2)+R*2
[ 8]  RP3←RP2*1.5
[ 9]  RP4←RP2×RP2
[10]  COS1←ZP÷RP2*0.5
[11]  COS2←COS1*2
[12]  R2Y20←RP2×¯1+3×COS2
[13]  R3Y30←RP3×COS1×¯3+5×COS2
[14]  R4Y40←RP4×3+COS2×¯30+35×COS2
[15]  Q200←R2Y20×(5÷○16)*0.5
[16]  Q300←R3Y30×(7÷○16)*0.5
[17]  Q400←R4Y40×(9÷○256)*0.5
[18]  Q20H←+/,VI×Q200×PP+PN
[19]  Q30H←+/,VI×Q300×PP+PN
[20]  Q40H←+/,VI×Q400×PP+PN
    ∇


    ∇ NORM AA;A;B;C;R;S;G;D;SS;GG
[ 1]  A←Z⌈|AA
[ 2]  B←Z⌊|AA
[ 3]  C←,|1-B÷A
```

```
[ 4]   D←,|A-B
[ 5]   R←÷⍴C
[ 6]   S←100×R×+/C
[ 7]   G←100×⌈/C
[ 8]   SS←R×+/D
[ 9]   GG←⌈∨D
[10]   ' '
[11]   'AFTER ';M;' ITERATIONS,'
[12]   'GREATEST  NORM FOR VARIABLE ',N,'  IS ';G;' PER CENT (';GG;')'
[13]   'AVERAGE   NORM FOR VARIABLE ',N,'  IS ';S;' PER CENT (';SS;')'
[14]   SPACE1
[15]   Z←|AA
[16]   ' DO WE CONTINUE ITERATING'
    ∇
```

```
    ∇  I NORMAIN MAT;M;G;S;A;B;R;D;GG;SS
[ 1]   M←|FREAD(400,I)
[ 2]   A←M⌈|MAT
[ 3]   B←M⌊|MAT
[ 4]   M←,|1-B÷A
[ 5]   D←,|A-B
[ 6]   R←÷⍴M
[ 7]   S←100×R×+/M
[ 8]   SS←R×+/D
[ 9]   G←100×⌈/M
[10]   GG←⌈/D
[11]   ' '
[12]   'GREATEST  NORM FOR VARIABLE ',N,'  IS ';G;' PERCENT (';GG;')'
[13]   'AVERAGE   NORM FOR VARIABLE ',N,'  IS ';S;' PERCENT (';SS;')'
[14]   ' '
    ∇
```

```
   ∇  Z←NORMDEN AA;I;C
[1]   C←DR×DR×DZ×○2
[2]   I←⍉(NZT,NR)⍴¯0.5+⍳NR
[3]   Z←C×+/,I×AA
   ∇
```

```
    ∇  NUCMAT;VI;Z;AA;DIS;PO;TO;T1;T2;T3;XO;C;DATA;DISP;MAT
[ 1]   VI←(DR×DZ×○2)×R←DR×⍉(NZT,NR)⍴¯0.5+⍳NR
[ 2]   Z←DZ×(NR,NZT)⍴¯1+⍳NZT
[ 3]   DISP←FREAD 11 33
[ 4]   ' NUCLEAR 'RMSRAD(PP+PN)
[ 5]   RMSTH←RMS
[ 6]   MAT←DATA
[ 7]   WAIT
[ 8]   ' PROTON 'RMSRAD PP
[ 9]   RMSPH←RMS
```

```
[10]  MAT←MAT,DATA
[11]  ' NEUTRON 'RMSRAD PN
[12]  RMSNH←RMS
[13]  MAT←MAT,DATA
[14]  WAIT
[15]  C←0.5×NZT+1
[16]  PO←0.25×PP[1;C-1]+PP[1;C]+PP[1;C+1]+PP[2;C]
[17]  PO←PO+0.25×PN[1;C-1]+PN[1;C]+PN[1;C+1]+PN[2;C]
[18]  KF←(1.5×PO×(○1)*2)*1÷3
[19]  TF←20.747×KF*2
[20]  TAU←0.6×TF
[21]  TO←¯1169.9
[22]  T1←585.6
[23]  T2←¯27.1
[24]  T3←9331
[25]  XO←0.34
[26]  BE←(0.6×TF)+(0.375×TO×PO)+T3×PO×PO÷16
[27]  BE←BE+(3÷80)×PO×KF×KF×(3×T1)+5×T2
[28]  K←(1.2×TF)+(2.25×TO×PO)+1.875×T3×PO*2
[29]  K←K+0.75×((3×T1)+5×T2)×PO×KF*2
[30]  AT←(TF÷3)-0.25×TO×PO×XO+0.5
[31]  AT←AT+(T2×PO×KF×KF÷6)-T3×PO×PO÷16
[32]  DISP←FREAD 11 34
[33]  DATA←7 1⍴PO,KF,TAU,TF,BE,K,AT
[34]  DATA←DISP,'F15.6'⎕FRMT DATA
[35]  AA←(⍴DATA)[2]
[36]  T←(1,AA)⍴AA↑'  CLEAR MATTER APPROXIMATION '
[37]  DATA←' ',T,' ',DATA,' '
[38]  ⎕←DATA
[39]  MAT←MAT,DATA
[40]  MAT FWRITE(4,ITIME)
[41]  WAIT
[42]  SPACE2
    ∇


    ∇ Z←PHI M;IP;JP
[ 1]  IP←M[1]
[ 2]  JP←M[2]
[ 3]  M←4×(IP-0.5)×M00÷((I00+IP-0.5)*2)∘.+(T×JP-J00)*2
[ 4]  Z←2×+/,P00×(DETK M)×(M×M00×DR)*0.5
[ 5]  M←4×(IP-0.5)×M10÷((I11+IP-0.5)*2)∘.+(T×JP-J00)*2
[ 6]  Z←Z++/,P10×(DETK M)×(M×M10×DR)*0.5
[ 7]  M←4×(IP-0.5)×M01÷((I00+IP-0.5)*2)∘.+(T×JP-J11)*2
[ 8]  Z←Z+4×+/,P01×(DETK M)×(M×M01×DR)*0.5
[ 9]  M←4×(IP-0.5)×M11÷((I11+IP-0.5)*2)∘.+(T×JP-J11)*2
[10]  Z←C×Z+2×+/,P11×(DETK M)×(M×M11×DR)*0.5
    ∇
```

```
    ∇  Z←PHIT M;IP;JP
[ 1]   IP←M[1]
[ 2]   JP←M[2]
[ 3]   M←4×(IP-0.5)×M00÷((I00+IP-0.5)*2)∘.+(T×JP-J00)*2
[ 4]   M[IP;(JP-1)]←0
[ 5]   Z←2×+/,P00×(DETK M)×(M×M00×DR)*0.5
[ 6]   M←4×(IP-0.5)×M10÷((I11+IP-0.5)*2)∘.+(T×JP-J00)*2
[ 7]   Z←Z++/,P10×(DETK M)×(M×M10×DR)*0.5
[ 8]   M←4×(IP-0.5)×M01÷((I00+IP-0.5)*2)∘.+(T×JP-J11)*2
[ 9]   Z←Z+4×+/,P01×(DETK M)×(M×M01×DR)*0.5
[10]   M←4×(IP-0.5)×M11÷((I11+IP-0.5)*2)∘.+(T×JP-J11)*2
[11]   Z←C×Z+2×+/,P11×(DETK M)×(M×M11×DR)*0.5
    ∇
```

```
    ∇  PLOTRAD AA;VI;A;ZO;ZP;R;MAT;ORDDENS;ORDRAD;NAME;L;B;DIS
[ 1]   VI←(DR×DZ×○2)×R←DR×⍉(NZT,NR)⍴¯0.5+⍳NR
[ 2]   A←+/,VI×AA
[ 3]   Z←DZ×(NR,NZT)⍴¯1+⍳NZT
[ 4]   ZO←(+/,Z×VI×AA)÷A
[ 5]   ZR←Z-ZO
[ 6]   R←((ZP*2)+R*2)*0.5
[ 7]   MAT←((NZT×NR),4)⍴0
[ 8]   MAT[;1]←,⍉(NZT,NR)⍴⍳NR
[ 9]   MAT[;2]←,(NR,NZT)⍴⍳NZT
[10]   MAT[;3]←,R
[11]   MAT[;4]←,AA
[12]   ORDDENS←⍋MAT[;4]
[13]   ORDRAD←⍋MAT[;3]
[14]   'ENTER NAME OF MATRIX'
[15]   NAME←⎕
[16]   'WHICH WAY DO YOU WANT '
[17]   '   1- NATURAL ORDERING'
[18]   '   2- DENSITY ORDERING'
[19]   '   3- RADIUS ORDERING'
[20]   L←⎕
[21]   'ADJUST PAPER'
[22]   B←⎕
[23]   SPACE5
[24]   'NORM IS ............................. ';A
[25]   'CENTER IS AT ........................ ';ZO
[26]   SPACE3
[27]   MAT←'I6 I6 F10.4 F10.4'⎕FRMT MAT
[28]   DIS←'     I     J    RADIUS    DENSITY'
[29]   →(L1,L2,L3)[L]
[30]  L1:NAME
[31]   SPACE2
[32]   DIS
[33]   SPACE1
[34]   MAT
[35]   SPACE5
[36]   →0
[37]  L2:MAT←MAT[ORDDENS;]
```

L

```
[38]  NAME
[39]  SPACE2
[40]  DIS
[41]  SPACE1
[42]  MAT
[43]  SPACE5
[44]  →0
[45] L3:MAT←MAT[ORDRAD;]
[46]  NAME
[47]  SPACE2
[48]  DIS
[49]  SPACE1
[50]  MAT
[51]  SPACE5
    ∇
```

```
    ∇  QUANTO L;I;NR;NZ;M;N;LL
[ 1]  LL←((L+2)×(L+3)×(5+2×L)÷24)-(L(L+3)÷2)÷4
[ 2]  QN←(LL,8)⍴0
[ 3]  I←1
[ 4]  NR←0
[ 5] L1:NZ←0
[ 6] L2:M←0
[ 7] L3:N←NZ+M+2×NR
[ 8]  QN[I;]←I,N,NR,NZ,M,(2×1+M≠0),0,0
[ 9]  I←I
[10]  I←I+1
[11]  M←M+1
[12]  →L3×⍳L>N
[13]  NZ←NZ+1
[14]  →L2×⍳M≠1
[15]  →L1×⍳L≥2×NR←NR+1
    ∇
```

```
    ∇  Y RADIAL Z;X;F;N;M;L;LL
[ 1]  SPACE3
[ 2] L4:'  ENTER DELTA R IN FERMIS'
[ 3]  DR←⎕
[ 4]  ' ENTER NO. OF POINTS IN R*DIRECTION'
[ 5]  NR←⎕
[ 6]  RMAT←(NR,(Y+1),(Z+1))⍴0
[ 7]  NRV←¯0.5+⍳NR
[ 8]  X←ALPHA×(DR×NRV)*2
[ 9]  F←(*X÷¯2)×(NRV÷○2)*0.5
[10]  N←0
[11] L1:M←0
[12] L2:L←LL←0
[13] L3:LL←LL+((-X)*L)×((N-L)!(N+M))÷(!L)
[14]  →L3×⍳N≥L←L+1
[15]  RMAT[;(M+1);(N+1)]←F×(X*M÷2)×LL×(2×ALPHA×(!N)÷(!N+M))*0.5
```

```
[16]  →L2×⍳Y≥M←M+1
[17]  →L1×⍳Z≥N←N+1
[18]  RMAT[NR;;]←0
[19]  ⎕←SUM←(○2)×(DR*2)×(+/RMAT*2)
[20]  '  IS THE NORMALIZATION CONDITION APPROXIMATLY SATISFIED'
[21]  →L4×GOIF'N'
[22]  SUM←(ρRMAT)ρSUM
[23]  RMAT←RMAT÷SUM*0.5
[24]  '  THE NORMALIZED RADIAL PART IS'
[25]  ⎕←(○2)×(DR*2)×(+/RMAT*2)
[26]  SPACE3
    ∇


    ∇ REC26;A;B
[ 1]  A←23 35ρ' '
[ 2]  B←' ',34ρ'.'
[ 3]  A[1;]←35↑'NEUTRON ENERGY',B
[ 4]  A[2;]←35↑'PROTON  ENERGY',B
[ 5]  A[3;]←35↑'TOTAL ENERGY',B
[ 6]  A[4;]←35↑'YUKAWA',B
[ 7]  A[5;]←35↑'2-BODY LOCAL',B
[ 8]  A[6;]←35↑'3-BODY LOCAL',B
[ 9]  A[7;]←35↑'KINETIC ENERGY',B
[10]  A[8;]←35↑'CURRENT CONTRIBUTION',B
[11]  A[9;]←35↑'EFFECTIVE MASS CONTRIBUTION',B
[12]  A[10;]←35↑'DIRECT COULOMB ENERGY',B
[13]  A[11;]←35↑'EXCHANGE COULOMB ENERGY',B
[14]  A[12;]←35↑'E3',B
[15]  A[13;]←35↑'E4 + E6',B
[16]  A[14;]←35↑'E5 + E7',B
[17]  A[15;]←35↑'E8',B
[18]  A[16;]←35↑'E911',B
[19]  A[17;]←35↑'E10 + E12',B
[20]  A[18;]←35↑'HO',B
[21]  A[19;]←35↑'HH',B
[22]  A[20;]←35↑'HV',B
[23]  A[21;]←35↑'TOTAL SINGLE-PARTICLE ENERGY',B
[24]  A[22;]←35↑'TOTAL HARTREE-FOCK ENERGY WITH EMC',B
[25]  A[23;]←35↑'TOTAL POTENTIAL ENERGY',B
[26]  A←A,' '
[27]  A FWRITE 11 26
[28]  'FMISC'FSAVE 11
    ∇


    ∇ REC32;A;B
[ 1]  B←' ',30ρ'.'
[ 2]  A←15 35ρ' '
[ 3]  A[1;]←35↑'NUMBER OF NUCLEONS',B
[ 4]  A[2;]←35↑'SEPERATION DISTANCE',B
[ 5]  A[3;]←35↑'CENTER OF MASS',B
```

```
[ 6]  A[4;]←35↑'LAMBDA 2',B
[ 7]  A[5;]←35↑'WANTED Q20',B
[ 8]  A[6;]←35↑'QUADRUPOLE MOMENT (FM×FM)',B
[ 9]  A[7;]←35↑'LAMBDA 3',B
[10]  A[8;]←35↑'WANTED Q30',B
[11]  A[9;]←35↑'OCTOPOLE MOMENT (FM×FM)',B
[12]  A[10;]←35↑'LAMBDA 4',B
[13]  A[11;]←35↑'WANTED Q40',B
[14]  A[12;]←35↑'HEXADUPOLE MOMENT (FM×FM)',B
[15]  A[13;]←35↑'NUCLEAR RMS RADIUS',B
[16]  A[14;]←35↑'PROTON RMS RADIUS',B
[17]  A[15;]←35↑'NEUTRON RMS RADIUS',B
[18]  A FWRITE 11 32
[19]  'FMISC'FSAVE 11
    ∇
```

```
    ∇ REC33;A;B
[ 1]  B←' ',35ρ'.'
[ 2]  A←7 35ρ' '
[ 3]  A[1;]←35↑'NORM',B
[ 4]  A[2;]←35↑'CENTER',B
[ 5]  A[3;]←35↑'MEAN RADIUS',B
[ 6]  A[4;]←35↑'MEAN OF RADIUS SQUARED',B
[ 7]  A[5;]←35↑'ROOT MEAN SQUARE RADIUS',B
[ 8]  A[6;]←35↑'EQUIVALENT UNIFORM RADIUS',B
[ 9]  A[7;]←35↑'STANDARD DEVIATION OF RADIUS',B
[10]  A FWRITE 11 33
[11]  'FMISC'FSAVE 11
    ∇
```

```
    ∇ REC34;A;B
[ 1]  B←' ',34ρ'.'
[ 2]  A←7 35ρ' '
[ 3]  A[1;]←35↑'DENSITY',B
[ 4]  A[2;]←35↑'FERMI MOMENTUM',B
[ 5]  A[3;]←35↑'AVERAGE KINETIC ENERGY',B
[ 6]  A[4;]←35↑'FERMI KINETIC ENERGY',B
[ 7]  A[5;]←35↑'BINDING ENERGY PER NUCLEON',B
[ 8]  A[6;]←35↑'NUCLEAR COMPRESSIBILITY',B
[ 9]  A[7;]←35↑'SYMMETRY ENERGY COEFFICIENT',B
[10]  A FWRITE 11 34
[11]  'FMISC'FSAVE 11
    ∇
```

```
    ∇ DIS RMSRAD AA;A;Z0;ZP;RP1;RP2;RMEAN;R2MEAN;RSD;EUR;T
[ 1]  A←+/,VI×AA
[ 2]  Z0←(+/,Z×VI×AA)÷A
[ 3]  ZP←Z-Z0
```

```
[ 4]   RP2←(ZP*2)+R*2
[ 5]   RP1←RP2*0.5
[ 6]   RMEAN←(+/,VI×RP1×AA)÷A
[ 7]   R2MEAN←(+/,VI×RP2×AA)÷A
[ 8]   RSD←(R2MEAN-RMEAN*2)*0.5
[ 9]   RMS←R2MEAN*0.5
[10]   EUR←RMS×(5÷3)*0.5
[11]   DATA←7 1⍴A,ZO,RMEAN,R2MEAN,RMS,EUR,RSD
[12]   DATA←DISP,'F15.4'⎕FRMT DATA
[13]   AA←(⍴DATA)[2]
[14]   T←(1,AA)⍴AA↑DIS,' RADII'
[15]   DATA←' ',T,' ',DATA,' '
[16]   ⎕←DATA
[17]   SPACE1
     ∇


     ∇   SAVEF;M;N;D;I
[ 1]   M←FREAD 11 24
[ 2]   N←FREAD 11 25
[ 3]   D←(⍴M)[1]
[ 4]   I←1
[ 5] L1:FUNTIE N[I]
[ 6]   M[I;]FTIE N[I]
[ 7]   →L1×⍳D≥I←I+1
[ 8]   ' '
[ 9]   'THE FILES ARE SAVED'
[10]   ' '
     ∇


     ∇   SDENHO;A;B;C;D;E
[ 1]   C←0.5+B←0.5+A←⍉(NZT,NR)⍴¯0.5+⍳NR
[ 2]   PP←PP×A←1÷A
[ 3]   PN←PN×A
[ 4]   PZP←((0 ¯1↓PP)+0 1↓PP)÷2
[ 5]   PZN←((0 ¯1↓PN)+0 1↓PN)÷2
[ 6]   PRP←((¯1 0↓PP)+1 0↓PP)÷2
[ 7]   PRN←((¯1 0↓PN)+1 0↓PN)÷2
[ 8]   TZP←PZP-TZP×E←0 ¯1↓A
[ 9]   TZN←PZN-TZN×E
[10]   TRP←(¯1 0↓B×A)×PRP-TRP×D←¯1 0↓(A÷C)*0.5
[11]   TRN←(¯1 0↓B×A)×PRN-TRN×D
[12]   SP←SP×D←A*3
[13]   SN←SN×D
     ∇


     ∇   SEEDENS;T;I;A;L;P;V;NAME;STOP
[ 1]   ⎕PP←5
[ 2]   SPACE3
```

```
[ 3]  V←50ρ'*'
[ 4]  '   DO YOU NEED TO SEE A LIST'
[ 5]  →L22×GOIF'N'
[ 6]  FNAMES,⍕((ρFNUMS),1)ρFNUMS
[ 7]  SPACE3
[ 8] L22:' ENTER FILE TIE NUMBER'
[ 9]  T←⎕
[10]  'ENTER NAME OF FILE'
[11]  NAME←⍞
[12]  '   ENTER NO. OF RECORD WE START AT'
[13]  I←⎕
[14]  I←I-1
[15]  'ENTER LAST RECORD WANTED'
[16]  STOP←⎕
[17] L1:I←I+1
[18]  A←FREAD(T,I)
[19] L2:SPACE2
[20]  V
[21]  ' RECORD ';I;' OF FILE ';NAME
[22]  SPACE2
[23]  ⎕←A
[24]  SPACE2
[25]  V
[26]  SPACE2
[27]  →L3×⍳STOP≤I
[28]  →L1
[29] L3:V
[30]  'STOP ENCOUNTERED-EXIT'
[31]  V
    ∇


    ∇ SEEFILE;T;I;A;L;P;V;NAME
[ 1]  SPACE3
[ 2]  V←50ρ'*'
[ 3]  '   DO YOU NEED TO SEE A LIST'
[ 4]  →L2×GOIF'N'
[ 5]  FNAMES,⍕((ρFNUMS),1)ρFNUMS
[ 6]  SPACE3
[ 7] L2:' ENTER FILE TIE NUMBER'
[ 8]  T←⎕
[ 9]  'ENTER NAME OF FILE'
[10]  NAME←⍞
[11]  '   ENTER NO. OF RECORD WE START AT'
[12]  I←⎕
[13]  I←I-1
[14] L1:I←I+1
[15]  A←FREAD(T,I)
[16]  ' DIMENSION OF RECORD ';I;' IS ';(ρA)
[17]  ' TYPE 1 TO DISPLAY,2 TO GO ON, → TO STOP'
[18]  L←⎕
[19]  →L1×⍳L=2
[20]  SPACE1
```

```
[21]  V
[22]  ' RECORD ';I;' OF FILE ';NAME
[23]  SPACE1
[24]  ⎕←A
[25]  SPACE1
[26]  V
[27]  SPACE1
[28]  →L1
    ∇


    ∇ SEEWF;T;I;A;L;P;V;NAME;STOP
[ 1] →⎕PP←5
[ 2]  SPACE3
[ 3]  V←50⍴'*'
[ 4]  '   DO YOU NEED TO SEE A LIST'
[ 5]  →L22×GOIF'N'
[ 6]  FNAMES,⍕((⍴FNUMS),1)⍴FNUMS
[ 7]  SPACE3
[ 8] L22:' ENTER FILE TIE NUMBER'
[ 9]  T←⎕
[10]  'ENTER NAME OF FILE'
[11]  NAME←⎕
[12]  '  ENTER NO. OF RECORD WE START AT'
[13]  I←⎕
[14]  I←I-1
[15]  'ENTER LAST RECORD WANTED'
[16]  STOP←⎕
[17] L1:I←I+1
[18]  A←FREAD(T,I)
[19]  →L2×⍳0≠+/,⍴A
[20]  SPACE2
[21]  ' DIMENSION OF RECORD ';I;' IS ';(⍴A)
[22]  ' TYPE 1 TO DISPLAY,2 TO GO ON, → TO STOP'
[23]  L←⎕
[24]  →L1×⍳L=2
[25] L2:SPACE2
[26]  V
[27]  ' RECORD ';I;' OF FILE ';NAME
[28]  SPACE2
[29]  'F7.4'⎕FRMT A[1;;]
[30]  SPACE1
[31]  'F7.4'⎕FRMT A[2;;]
[32]  SPACE2
[33]  V
[34]  SPACE2
[35]  →L3×⍳STOP≤I
[36]  →L1
[37] L3:V
[38]  'STOP ENCOUNTERED-EXIT'
[39]  V
    ∇
```

```
    ∇  SETNOS;I
[ 1]   QNN←FREAD 16 0
[ 2]   QNP←FREAD 15 0
[ 3]   OCCP←QNP[;6]
[ 4]   OCCN←QNN[;6]
[ 5]   MP←QNP[;5]
[ 6]   MN←QNN[;5]
[ 7]   EP←QNP[;7]
[ 8]   EN←QNN[;7]
[ 9]   I←FREAD 11 29
[10]   NN←I[1]
[11]   NP←I[2]
[12]   I←FREAD 11 30
[13]   NZ←I[1]
[14]   NZT←I[2]
[15]   DZ←I[3]
[16]   NR←I[4]
[17]   DR←I[5]
[18]   NMN←I[6]
[19]   NMP←I[7]
    ∇


    ∇  SETYC;A;AA;BB;D;FL;GG;H;I;IH;IV;MI;NP;R;RE;RO;RR;V;Z;Y
[ 1]   SPACE3
[ 2]   '  ENTERING SETYC FUNCTION'
[ 3]   A←0.45979
[ 4]   'IS THE VALUE OF THE RANGE OF THE YUKAWA FORCE TO'
[ 5]   'BE A= ';A;' FM'
[ 6]   →L1×GOIF'Y'
[ 7]   'ENTER DESIRED VALUE'
[ 8]   A←⎕
[ 9]  L1:FL←0
[10]   D←-MI÷DR×DR×(¯0.25+MI×MI←⍳NR-1)*0.5
[11]   V←(NR,NR)⍴0
[12]   I←2
[13]  L2:V[I;I-1]←V[(I-1);I]←D[I-1]
[14]   →L2×⍳NR≥I←I+1
[15]   IV←(NR,NR)⍴1,(NR⍴0)
[16]   Z←-1÷DZ*2
[17]   H←(NZT,NZT)⍴0,Z,((NZT-2)⍴0),Z
[18]   IH←(NZT,NZT)⍴1,(NZT⍴0)
[19]   A←1÷2×A*2
[20]  L3:AA←A+((○1)÷2×DZ×NZ-1)*2
[21]   R←(4×NR>7)++/1 2 3×NR=5 6 7
[22]   Z←(14.9309,18.0711,21.2116,(○NR))[R]
[23]   BB←A+(Z÷DR×NR-0.5)*2
[24]   GG←(0.5×(AA+BB)×(AA×BB)*0.5)*0.5
[25]   RO←GG+((GG×GG)-AA×BB)*0.5
[26]   RE←GG-((GG×GG)-AA×BB)*0.5
[27]   R←A+2÷DR×DR
[28]   Z←A+2÷DZ×DZ
[29]   RR←((RE-R)×IV)-V
```

```
[30]  RR FWRITE(11,0+8×FL)
[31]  RR←((RO-R)×IV)-V
[32]  RR FWRITE(11,1+8×FL)
[33]  RR←((RE-Z)×IH)-H
[34]  RR FWRITE(11,2+8×FL)
[35]  RR←((RO-Z)×IH)-H
[36]  RR FWRITE(11,3+8×FL)
[37]  RR←⊖((RE+R)×IV)+V
[38]  RR FWRITE(11,4+8×FL)
[39]  RR←⊖((RO+R)×IV)+V
[40]  RR FWRITE(11,5+8×FL)
[41]  RR←⊖((RE+Z)×IH)+H
[42]  RR FWRITE(11,6+8×FL)
[43]  RR←⊖((RO+Z)×IH)+H
[44]  RR FWRITE(11,7+8×FL)
[45]  →L4×⍳FL≠0
[46]  FL←1
[47]  A←0
[48]  →L3
[49] L4:'FMISC'FSAVE 11
[50]  '    LEAVING SETYC FUNCTION'
[51]  SPACE3
    ∇


    ∇ SPACE
[1]  SPACE1←' '
[2]  SPACE2←2 1⍴' '
[3]  SPACE3←3 1⍴' '
[4]  SPACE5←5 1⍴' '
[5]  SPACE10←10 1⍴' '
    ∇


     ∇  STDHF;I;IM;J;ITS
[  1]  SPACE5
[  2]  ' THIS IS THE MAIN PROGRAM FOR THE STATIC AND TIME-DEPENDENT'
[  3]  ' HARTREE-FOCK CALCULATIONS'
[  4]  SPACE2
[  5]  →L5×⍳1=∨/11=0,FNUMS
[  6]  'FMISC'FTIE 11
[  7] L5:' DO WE NEED TO TIE THE FILES'
[  8]  →L10×GOIF'N'
[  9]  TIEF
[ 10] L10:' DO WE NEED TO CALCULATE THE STARTING WAVE FUNCTIONS'
[ 11]  '( ANISOTROPIC HARMONIC OSCILLATOR, SINGLE CENTER )'
[ 12]  →L20×GOIF'N'
[ 13]  INITIAL
[ 14]  ITIME←0
[ 15]  PNOLD←F1
[ 16]  PTOLD←T1
[ 17]  NNOLD←F2
```

```
[ 18]  NTOLD←T2
[ 19]  →L30
[ 20] L20:'ENTER THE FILE NAME WHERE THE PROTON WAVE FUNCTIONS ARE'
[ 21]  ' STORED'
[ 22]  PNOLD←⎕
[ 23]  ' ENTER THE TIE NO.'
[ 24]  PTOLD←⎕
[ 25]  ' ENTER THE FILE NAME WHERE THE NEUTRON WAVE FUNCTIONS ARE '
[ 26]  ' STORED'
[ 27]  NNOLD←⎕
[ 28]  ' ENTER THE TIE NO.'
[ 29]  NTOLD←⎕
[ 30]  ' DO WE NEED TO TIE THESE FILES'
[ 31]  →L28×GOIF'N'
[ 32]  PNOLD FTIE PTOLD
[ 33]  NNOLD FTIE NTOLD
[ 34] L28:SETNOS
[ 35]  PTOLD DENS NTOLD
[ 36] L30:STODENS
[ 37]  ' DO WE NEED TO COPY ',PNOLD,' ON WFEVENP'
[ 38]  →L40×GOIF'N'
[ 39]  ' ENTER NO. OF WAVE FUNCTIONS IN FILE ',PNOLD
[ 40]  IM←⎕
[ 41]  188 COPYF PTOLD
[ 42] L40:' DO WE NEED TO COPY ',NNOLD,' ON WFEVENN'
[ 43]  →L50×GOIF'N'
[ 44]  ' ENTER NO. OF WAVE FUNCTIONS IN FILE ',NNOLD
[ 45]  IM←⎕
[ 46]  288 COPYF NTOLD
[ 47] L50:' ENTER THE INITIAL TIME ITERATION NO. ( ITIME)'
[ 48]  RAW←(NN+NP-1)÷NN+NP
[ 49]  ITIME←⎕
[ 50]  ' ENTER THE SIZE OF THE DESIRED TIME STEP ( TSTEP ) IN'
[ 51]  ' UNITS OF E¯21 SECONDS'
[ 52]  TSTEP←⎕
[ 53]  TS←0.759627×TSTEP
[ 54]  ' ENTER TYPE OF CALCULATION (TTYPE=0 FOR SHF; 1 FOR TDHF)'
[ 55]  TTYPE←⎕
[ 56]  MFLAG←1
[ 57]  ' DO WE RUN SETYC'
[ 58]  →L75×GOIF'N'
[ 59] L70:SETYC
[ 60] L75:'ENTER NO. OF LOOPS PER MAIN ITERATION (1 OR 2)'
[ 61]  LOOP150←⎕
[ 62]  LOOP150←1⌈2⌊LOOP150
[ 63]  DELENO←1111
[ 64]  'ENTER PRINTING PRECISION'
[ 65]  ⎕PP←⎕
[ 66]  YUKAWA
[ 67]  COULOMB
[ 68]  NUCMAT
[ 69]  MPMEAS
[ 70]  ENERGYT
[ 71]  EEN←EN
```

```
[ 72]  FEP←EP
[ 73]  ' DO WE COMPUTE THE SINGLE PARTICLE ENERGIES'
[ 74]  →L80×GOIF'N'
[ 75]  NTOLD ENERGY PTOLD
[ 76]  EN←ENSPN
[ 77]  EP←ENSPP
[ 78] L80:ITS←0
[ 79] L100:' MAIN RUN WITH ITIME=';ITIME
[ 80]  MPFIXL
[ 81]  I←1+ITIME-2×⌊0.5×ITIME
[ 82]  PTN←(199,188)[I]
[ 83]  PTO←(188,199)[I]
[ 84]  NTN←(299,288)[I]
[ 85]  NTO←(288,299)[I]
[ 86]  TS←TS÷LOOP150*2
[ 87] L150:TERMS
[ 88]  TS←TS×LOOP150
[ 89]  PTN EVOLVEP PTO
[ 90]  NTN EVOLVEN NTO
[ 91]  NTN GRAMSCH PTN
[ 92]  PTN DENS NTN
[ 93]  →L200×⍳(MFLAG=0)∨LOOP150=1
[ 94]  MFLAG←0
[ 95]  HALFDEN
[ 96]  →L150
[ 97] L200:MAINORM
[ 98]  ITIME←ITIME+1
[ 99]  STODENS
[100]  MFLAG←1
[101]  YUKAWA
[102]  COULOMB
[103]  NUCMAT
[104]  MPMEAS
[105]  ENERGYT
[106]  'DO WE COMPUTE THE SINGLE PARTICLE ENERGIES'
[107]  →L205×GOIF'N'
[108]  NTN ENERGY PTN
[109]  'DO WE LOOK AT THE SINGLE-PARTICLE ENERGY ORDERING'
[110]  →L203×GOIF'N'
[111]  ENORDER ITIME
[112]  EPORDER ITIME
[113]  →L205
[114] L203:DELENN←+/OCCN×(|(ENSPN*2)-EN*2)*0.5
[115]  DELENP←+/OCCP×(|(ENSPP*2)-EP*2)*0.5
[116]  EN←ENSPN
[117]  EP←ENSPP
[118]  QNN[;7]←EN
[119]  QNP[;7]←EP
[120]  QNN FWRITE(16,ITIME)
[121]  QNP FWRITE(15,ITIME)
[122] L205:ENCONV
[123]  'DO WE SAVE THE FILES (LAST ITERATION SAVED WAS ';ITS;')'
[124]  →L210×GOIF'N'
[125]  ITS←ITIME-1
```

```
[126]  SAVEF
[127]  'FMISC'FSAVE 11
[128]  ⎕SAVE'PART2'
[129] L210:' WE ARE AT ITERATION NO. ';ITIME;' , DO WE GO ON'
[130]  SPACE2
[131]  '*****************************************'
[132]  →L300×GOIF'N'
[133]  'DO YOU WANT TO CHANGE NO. OF LOOPS IN MAIN ITERATION'
[134]  →L100×GOIF'N'
[135]  'ENTER NEW VALUE'
[136]  LOOP150←⎕
[137]  →L100
[138] L300:' NEW PROTON WAVE FUNCTIONS ARE TIED TO ';PTN
[139]  ' NEW NEUTRON WAVE FUNCTIONS ARE TIED TO ';NTN
[140]  '********************DO ANALYSIS****************************'
[141]  SPACE5
     ∇
```

```
     ∇  STODENS
[ 1]   PP FWRITE 400 1
[ 2]   PN FWRITE 400 2
[ 3]   PRP FWRITE 400 3
[ 4]   PRN FWRITE 400 4
[ 5]   PZP FWRITE 400 5
[ 6]   PZN FWRITE 400 6
[ 7]   JRP FWRITE 400 7
[ 8]   JRN FWRITE 400 8
[ 9]   JZP FWRITE 400 9
[10]   JZN FWRITE 400 10
[11]   TRP FWRITE 400 11
[12]   TRN FWRITE 400 12
[13]   TZP FWRITE 400 13
[14]   TZP FWRITE 400 13
[15]   TZN FWRITE 400 14
[16]   SP FWRITE 400 15
[17]   SN FWRITE 400 16
     ∇
```

```
     ∇  SUMDENS;A;B;C;D;E
[ 1]   C←0.5+B←0.5+A←⍉(NZT,NR)⍴¯0.5+⍳NR
[ 2]   PP←PP×A←1÷A
[ 3]   PN←PN×A
[ 4]   PZP←((0 ¯1↓PP)+0 1↓PP)÷2
[ 5]   PZN←((0 ¯1↓PN)+0 1↓PN)÷2
[ 6]   PRP←((¯1 0↓PP)+1 0↓PP)÷2
[ 7]   PRN←((¯1 0↓PN)+1 0↓PN)÷2
[ 8]   TZP←PZP-TZP×E←0 ¯1↓A
[ 9]   TZN←PZN-TZN×E
[10]   TRP←(¯1 0↓B×A)×PRP-TRP×D←¯1 0↓(A÷C)*0.5
[11]   TRN←(¯1 0↓B×A)×PRN-TRN×D
```

```
[12]  SP←SP×D←A⋆3
[13]  SN←SN×D
[14]  JZN←JZN×E
[15]  JRN←JRN×D←¯1 0↓((B÷C)⋆0.5)×A
[16]  JZP←JZP×E
[17]  JRP←JRP×D
    ∇


   ∇  TDENS;I
[1]   I←NORMDEN PP
[2]   ' '
[3]   ' NORM OF PP IS ';I;' WHILE NP IS ';NP
[4]   I←NORMDEN PN
[5]   ' NORM OF PN IS ';I;' WHILE NN IS ';NN
   ∇


    ∇  TERMS;A;B;B1;BO;I;RO;R3;R1;X1;X2;R2Y20;R2Y30;R2Y40;X;VI;Y;Z
[ 1]   SPACE3
[ 2]   'ENTERING TERMS'
[ 3]   DRM2←÷DR×DR
[ 4]   DZM2←÷DZ×DZ
[ 5]   A←FREAD 11 22
[ 6]   B←FREAD 11 23
[ 7]   KQ←B[2]+B[3]
[ 8]   KNQ←B[2]÷KQ
[ 9]   B1←RAW×B[1]
[10]   BO←RAW×B[4]
[11]   I←⍳NR-1
[12]   RO←⍉(NZT,NR-1)⍴I÷I-0.5
[13]   R3←⍉(NZT,NR-1)⍴(I-0.5)÷I+0.5
[14]   R1←⍉(NZT,NR-1)⍴I÷I+0.5
[15]   Z0←(1,NZT)⍴0
[16]   X1←KQ×(TRN+RO×PRN)+KNQ×TRP+RO×PRP
[17]   X2←Z0⍪KQ×((R3×TRN)+R1×PRN)+KNQ×(R3×TRP)+R1×PRP
[18]   DON←DRM2×BO+(KQ×SN+KNQ×SP)+X2+X1⍪Z0
[19]   DON[1;]←KQ×(TRN[1;]+2×PRN[1;])+KNQ×TRP[1;]+2×PRP[1;]
[20]   DON[1;]←DRM2×BO+DON[1;]+KQ×SN[1;]+KNQ×SP[1;]
[21]   X1←KQ×(TRP+RO×PRP)+KNQ×TRN+RO×PRN
[22]   X2←Z0⍪KQ×((R3×TRP)+R1×PRP)+KNQ×(R3×TRN)+R1×PRN
[23]   DOP←DRM2×BO+(KQ×SP+KNQ×SN)+X2+X1⍪Z0
[24]   DOP[1;]←KQ×(TRP[1;]+2×PRP[1;])+KNQ×TRN[1;]+2×PRN[1;]
[25]   DOP[1;]←DRM2×BO+DOP[1;]+KQ×SP[1;]+KNQ×SN[1;]
[26]   HON←(A[1]×PP)+(PN×A[1]-A[2])+(A[4]×UYP)+A[5]×UYN
[27]   HON←HON+A[3]×(PP×PN)+PP×PP+PN
[28]   MPTERMS
[29]   JX←+/,X←2×Q200×Q20H-Q2H
[30]   JY←+/,Y←2×Q300×Q30H-Q3H
[31]   JZ←+/,Z←2×Q400×Q40H-Q4H
[32]   HOP←UCP+(-A[6]×PP⋆1÷3)+(A[1]×PN)+(PP×A[1]-A[2])+A[4]×UYN
[33]   HOP←HOP+(A[5]×UYP)+A[3]×(PP×PN)+PN×PN+PP
```

```
[34]   JH←+/,HOP+HON
[35]   X←X×LAMBD2H×|JH÷JX
[36]   Y←Y×LAMBD3H×|JH÷JY
[37]   Z←Z×LAMBD4H×|JH÷JZ
[38]   HON←HON+X+Y+Z
[39]   HOP←HOP+X+Y+Z
[40]   UCP←UYP←UYN←1
[41]   I←⍳NR-1
[42]   R3←R0⋆0.5
[43]   R0←⍉(NZT,NR-1)⍴I÷(¯0.25+I×I)⋆0.5
[44]   APP←APN←(2,(NR-1),NZT)⍴0
[45]   APN[1;;]←-DRM2×R0×B1+KQ×PRN+KNQ×PRP
[46]   APN[2;;]←DRM2×R3×KQ×JRN+KNQ×JRP
[47]   APP[1;;]←-DRM2×R0×B1+KQ×PRP+KNQ×PRN
[48]   APP[2;;]←DRM2×R3×KQ×JRP+KNQ×JRN
[49]   PRP←PRN←JRP←JRN←1
[50]   II←⍉(NZT,NR)⍴1÷(¯0.5+⍳NR)⋆2
[51]   CON1←DRM2×II×B1+KQ×PN+KNQ×PP
[52]   COP1←DRM2×II×B1+KQ×PP+KNQ×PN
[53]   PP←PN←TRP←TRN←SP←SN←1
[54]   X1←KQ×PZN+TZN+KNQ×PZP+TZP
[55]   R0←(NR,1)⍴0
[56]   BON←DZM2×B0+(X1,R0)+R0,X1
[57]   X1←KQ×PZP+TZP+KNQ×PZN+TZN
[58]   BOP←DZM2×B0+(X1,R0)+R0,X1
[59]   TZP←TZN←X2←X1←1
[60]   BPN←BPP←(2,NR,NZT-1)⍴0
[61]   BPN[1;;]←-DZM2×B1+KQ×PZN+KNQ×PZP
[62]   BPN[2;;]←DZM2×KQ×JZN+KNQ×JZP
[63]   BPP[1;;]←-DZM2×B1+KQ×PZP+KNQ×PZN
[64]   BPP[2;;]←DZM2×KQ×JZP+KNQ×JZN
[65]   PZP←PZN←JZP←JZN←1
[66]   'LEAVING TERMS'
[67]   SPACE1
[68]   ⎕←+/,X
[69]   ⎕←+/,Y
[70]   ⎕←+/,Z
     ∇
```

```
     ∇ TIEF;M;N;D;I
[ 1]   SPACE2
[ 2]   M←FREAD 11 24
[ 3]   N←FREAD 11 25
[ 4]   D←(⍴M)[1]
[ 5]   I←1
[ 6] L1:M[I;]FTIE N[I]
[ 7]   →L1×⍳D≥I←I+1
[ 8]   N←((⍴FNUMS),1)⍴FNUMS
[ 9]   'THE FOLLOWING ARE THE FILES THAT ARE NOW TIED'
[10]   ' '
[11]   FNAMES,⍕N
[12]   SPACE2
     ∇
```

```
  ∇ UNTIEF;N
[1]  ' '
[2]  N←FREAD 11 25
[3] L1:FUNTIE N
[4]  N←((⍴FNUMS),1)⍴FNUMS
[5]  'THE FOLLOWING ARE THE FILES THAT ARE NOW TIED'
[6]  '    '
[7]  FNAMES,⍕N
[8]  ' '
  ∇
```

```
  ∇ WAIT;A
[1]  A←⎕
  ∇
```

```
  ∇ WFN A;NR;NZ;M
[1]  NR←A[1]+1
[2]  NZ←A[2]+1
[3]  M←A[3]+1
[4]  WF[1;;]←RMAT[;M;NR]∘.×ZMAT[NZ;]
[5]  WF[;;(1,NZT)]←0
[6]  WF←WF×WFNORM WF
  ∇
```

```
  ∇ Z←WFNORM AA;NORM
[1]  NORM←(○2)×DR×DR×DZ×+/,AA*2
[2]  Z←NORM*¯0.5
  ∇
```

```
   ∇ YUKAWA;YFLAG;S;AA;BB;RIH;M;ML;R0;R1;R2;R3;R4;R5;R6;R7;A;Z;N
[ 1]  SPACE3
[ 2]  N←' AA '
[ 3]  '   ENTERING YUKAWA FUNCTION'
[ 4]  R0←FREAD 11 0
[ 5]  R1←FREAD 11 1
[ 6]  R2←FREAD 11 2
[ 7]  R3←FREAD 11 3
[ 8]  R4←FREAD 11 4
[ 9]  R5←FREAD 11 5
[10]  R6←FREAD 11 6
[11]  R7←FREAD 11 7
[12]  A←FREAD 11 16
[13]  YFLAG←0
[14]  RIH←⍉(NZT,NR)⍴(DR×¯0.5+⍳NR)*0.5
[15]  →L1×⍳ITIME≠0
[16]  AA←A×A×S←RIH×FN×A×○4
```

```
[17]  ML←20
[18]  →L2
[19] L1:UYN←FREAD 11 28
[20]  S←RIH×PN×A×4×○1
[21]  AA←RIH×UYN
[22]  ML←2
[23] L2:' SUGGESTED NO. OF ITERATIONS IS ';ML
[24]  Z←|AA
[25]  M←0
[26] L3:BB←(S+R1+.×AA)+.×R7
[27]  AA←R5+.×(S+BB+.×R3)
[28]  BB←(S+R0+.×AA)+.×R6
[29]  AA←R4+.×(S+BB+.×R2)
[30]  AA[;1]←AA[;NZT]←0
[31]  AA[NR;]←0
[32]  M←M+2
[33]  NORM AA
[34]  →L3×GOIF'Y'
[35]  →L4×⍳YFLAG=1
[36]  YFLAG←1
[37]  UYN←AA÷RIH
[38]  UYN FWRITE 11 28
[39]  S←RIH×PP×A×○4
[40]  →L5×⍳ITIME=0
[41]  UYP←FREAD 11 27
[42]  AA←RIH×UYP
[43]  →L2
[44] L5:AA←S×A*2
[45]  →L2
[46] L4:UYP←AA÷RIH
[47]  UYP FWRITE 11 27
[48]  '  LEAVING YUKAWA FUNCTION'
[49]  SPACE3
    ∇


    ∇  ZED L;X;C;E;I;SUM;NZV;V
[ 1]  SPACE3
[ 2] L2:'  ENTER DELTA Z IN FERMIS'
[ 3]  DZ←⎕
[ 4]  'ENTER NO. OF POINTS IN  POSITIVE (NEGATIVE) DIRECTION (NZ)'
[ 5]  NZ←⎕
[ 6]  NZT←1+2×NZ
[ 7]  NZV←(⍳NZT)-NZ+1
[ 8]  X←DZ×NZV×GAMMA*0.5
[ 9]  ZMAT←((L+1),NZT)⍴0
[10]  C←(GAMMA÷(○1))*0.25
[11]  E←*(X*2)÷¯2
[12]  ZMAT[1;]←C×E
[13]  →L3×⍳L=0
[14]  ZMAT[2;]←C×E×X×2*0.5
[15]  →L3×⍳L<2
[16]  I←1
```

```
[17] L1:I←I+1
[18]  V←I-1
[19]  ZMAT[(I+1);]←(((2⋆0.5)×X×ZMAT[I;])-(V⋆0.5)×ZMAT[V;])÷I⋆0.5
[20]  →L1×⍳L>I
[21]  ZMAT[;1]←ZMAT[;NZT]←0
[22] L3:⎕←SUM←DZ×(+/ZMAT⋆2)
[23]  '   IS THE NORMALIZATION CONDITION APPROXIMATLY SATISFIED'
[24]  →L2×GOIF'N'
[25]  SUM←⍉(NZT,L+1)⍴SUM
[26]  ZMAT←ZMAT÷SUM⋆0.5
[27]  'THE NORMALIZED ZED PART IS'
[28]  ⎕←DZ×(+/ZMAT⋆2)
[29]  SPACE5
    ∇
```