Effective charges and isoscalar shifts in the linearized Hartree-Fock model*

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A simple method based on a linearized Hartree-Fock technique is proposed to calculate effective charges and isoscalar nuclear shifts. As an application, the change in rms radii near closed shell nuclei is calculated using a Skyrme interaction.

[NUCLEAR STRUCTURE Hartree-Fock calculation of effective charge, isoscalar nuclear shift, Skyrme interaction.]

In recent years there has been an accumulation of experimental data[1] on the change of nuclear bulk properties induced by a polarizing valence particle (or hole). For a microscopic description of these isoscalar nuclear shifts, the Hartree-Fock (HF) and random phase approximation (RPA) techniques are mostly used. The description in terms of HF generally involves a calculation of the A and $A+1$ systems and a comparison of the results. Such a treatment, however, encounters difficulties caused by the non-time-reversal invariance of the odd-A system.[2,3] In RPA calculations, one couples the odd particle to the vibrational states of the core.[4] There one faces difficulties in treating correctly the continuum of the unbound orbitals or in conserving the particle number in open shell nuclei. These shortcomings can be avoided by using a linearized HF model,[5,6] whose main advantage consists in *requiring information on the properties of the doubly even system only* (at equilibrium and slightly away from it). In the present note we show how a Taylor expansion technique in terms of constrained HF wave functions can be used to calculate isoscalar nuclear shifts and effective charges. As a numerical application we present a calculation of the change in rms radii for a few A and $A\pm1$ nuclei near closed shell and compare our results with experiments.

In the HF theory with a density dependent or density independent interaction, one defines the HF Hamiltonian W by the variation of the total energy E with respect to the single particle (s.p.) density matrix ρ, i.e., $\delta E = \mathrm{Tr}(W\delta\rho)$. The single particle energies corresponding to the s.p. wave functions ϕ_i are given by $W\phi_i = \epsilon_i\phi_i$. The total energy of an $A+1$ system with a particle in the state $|p\rangle$ is then given by[7]

$$E_{A+1} = E_A + \epsilon_p . \tag{1}$$

We are now interested in calculating the effective charge associated with the multipole operator $\hat{Q}_\lambda = \sum_i Q(i)$ with $Q(i) = r_i^2, r_i^2 Y_{20}(i), r_i^3 Y_{30}(i)$, for monopole, quadrupole, octupole transitions, etc. We then define a collective coordinate $q = \langle\phi|\hat{Q}|\phi\rangle$ where $|\phi\rangle$ represents the total HF wave function.

Let us denote by q_A the expectation value of $\hat{Q}_A$ at equilibrium in the A system, then

$$(\partial E_{A+1}/\partial q)q_A = (\partial\epsilon_p/\partial q)q_A ; \quad (\partial E_A/\partial q)q_A = 0 . \tag{2}$$

We now expand the left hand side in a Taylor series around q_{A+1}[5] where q_{A+1} denotes the expectation value of $\hat{Q}_{A+1}$ in the $A+1$ system:

$$(\partial E_{A+1}/\partial q)q_A = (q_A - q_{A+1})(\partial^2 E_{A+1}/\partial q^2)q_{A+1} \tag{3}$$

and express the difference by

$$\Delta q \equiv q_{A+1} - q_A = -\frac{(\partial\epsilon_p/\partial q)q_A}{(\partial^2 E/\partial q^2)q_{A+1}} . \tag{4}$$

For heavier nuclei, one can neglect in $\partial^2 E/\partial q^2$ the difference between the A and $A+1$ systems which amounts to $(\partial^2\epsilon_p/\partial q^2)q_A$; one then obtains

$$\Delta q = -\frac{(\partial\epsilon_p/\partial q)q_A}{(\partial^2 E_A/\partial q^2)q_A} . \tag{5}$$

The effective charge can now be defined as

$$e_{\mathrm{eff}}^{(p)} = \Delta q/q_p \quad \text{with } q_p = \langle p|Q|p\rangle . \tag{6}$$

In order to calculate Δq, the derivatives $\partial\epsilon/\partial q$ can be obtained by performing several constrained HF calculations with $\hat{Q}$ as the constraining operator for various values of the Lagrange parameter λ in the vicinity of $\lambda = 0$:

$$(W - \lambda Q)\phi_i(q) = \epsilon_i^{\mathrm{CHF}}(q)\phi_i(q) \tag{7}$$

with $q = q(\lambda)$. One should not confuse ϵ^{CHF} with the s.p. energies needed above [cf., Eqs. (4) and (5)]: the ϵ^{CHF} are affected by the hole-hole and particle-particle matrix elements of $\hat{Q}$ whereas only the

TABLE I. Calculated and experimental change of rms radii.

Nuclei	ΔR (10^{-3} fm) Exp.	Calc.	Calc. (ϵ^{CHF})
^{207}Pb–^{208}Pb	6.3	6.6	22.3
^{209}Bi–^{208}Pb	14.5	8.6	25.0
^{89}Y–^{90}Zr	27 ±7	14.3	103.8

particle-hole matrix elements of $\hat{Q}$ are relevant in distorting the system. This is clear since Eq. (7) is a direct result of the variational principle

$$\delta_{ph}\langle\phi(q)|(H-\lambda\hat{Q})a_p^\dagger a_h|\phi(q)\rangle=0\,.$$

The Hamiltonian W is therefore diagonalized in the subspace of occupied and unoccupied s.p. wave functions, respectively. Denoting by m,n particle states and by i and j hole states, the new s.p. matrix elements are then given by

$$\langle i|W|j\rangle=\epsilon_i\delta_{ij}\,,\quad \langle m|W|n\rangle=\epsilon_m\delta_{mn}$$

with

$$\langle i|W-\lambda Q|n\rangle=0\,.$$

The usefulness of the above formalism can be illustrated by a calculation of the change in rms radii near closed shell nuclei. The constraining operator is $\hat{Q}=\sum_i r_i^2$ and we shall adopt the density and momentum dependent Skyrme VI interaction[8] which gives, among the other parametrizations of Skyrme's interaction, the best single particle energies near the Fermi surface. The calculations are performed using a basis of more than 20 harmonic oscillator shells. For an accurate calculation of $\partial\epsilon/\partial q$ it became sufficient to perform five constrained HF calculations with $\lambda=0.0;\pm0.02;\pm0.04$.

Table I lists the change in rms radii between ^{208}Pb, ^{90}Zr, and neighboring odd-A nuclei.[1,9] The experimental values originate from a two-parameter Fermi-type charge distribution with the exception of the ^{209}Bi–^{208}Pb data which results from an analysis of the charge density using the Friar-Negele method.[10] In general one should view the agreement as very satisfactory especially if one considers the model dependence of the experimental results. The importance of using the proper s.p. energies is well illustrated by the comparison between columns 2 and 3 of Table I where ϵ and ϵ^{CHF} are used, respectively.

In conclusion the comparison of the linearized HF results with the available experimental data indicates that this simple method provides a useful tool for the calculation of isoscalar properties at least in the case of the monopole operator near doubly closed shells. Further applications of the method to multipole operators of higher order are in progress.

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