CAN WE OBTAIN NUCLEAR BINDING AND DEFORMATION ENERGIES IN A SELFCONSISTENT WAY WITHOUT DOING HARTREE-FOCK CALCULATIONS?

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The validity of the shell-correction (SC) method /1,2/ has been tested extensively in constrained Hartree-Fock (HF) calculations using effective interactions of the Skyrme type /3,4/. The total HF energy is expanded around the average part of the selfconsistent density matrix ϱ (thus writing $\varrho = \tilde{\varrho} + \delta\varrho$):

$$E_{HF}[\varrho] = E_{HF}[\tilde{\varrho}] + \delta_1 E + \delta_2 E \,. \qquad (1)$$

Here $E_{HF}[\tilde{\varrho}]$ represents the average binding energy which is parametrized in the liquid drop model; $\delta_1 E$ is the first order shell-correction defined in the usual way /1,2/ in terms of the eigenvalues of the averaged HF potential (which may be parametrized by the shell model potential). The term $\delta_2 E$ contains contributions of second and higher orders in $\delta\varrho$ and is neglected in the usual SC approach. - It was shown numerically /3,4/ that the series (1) converges extremely well; the energy $\delta_2 E$ is not larger than ~1-3 MeV in medium and heavy nuclei. It was especially found /4/ that if $\tilde{\varrho}$ is iterated to selfconsistency, $\delta_2 E$ is less than ~0.6 MeV and practically constant as function of both deformation and nucleon numbers, even for nuclei as light as O^{16} and Ca^{40}. - This result provides a strong motivation for a method in which only the average binding energy and the average field are calculated selfconsistently with some effective interaction (and a constraint on the deformation), and the shell-correction is added as a perturbation, using the selfconsistent average field obtained in the first step. For the average selfconsistency problem, we propose to use the extended Thomas-Fermi (ETF) model, in which the total energy for a given one-body potential V(r) is obtained directly in terms of V(r) and its derivatives /5/. Note that the pure TF approximation is not sufficient; the semiclassical corrections to it contribute up to ~100 MeV in a heavy nucleus. In the Strutinsky averaging method one automatically includes these corrections. It has been checked /6/ that for realistic (spherical and deformed) Woods-Saxon potentials, including a spin-orbit part, the ETF energies agree with the Strutinsky averaged energies within ~1-2 MeV. - Instead of solving a differential equation for the density $\tilde{\varrho}(r)$, we iterate both V(r) and $\tilde{\varrho}(r)$ until selfconsistency is reached. Hereby an exponential tail is added to the semiclassical $\tilde{\varrho}(r)$ which is only defined inside the classically allowed region. The kinetic energy density is expanded in terms of $\tilde{\varrho}(r)$. We have recently shown /7/ that the average kinetic energy in a Woods-Saxon potential can be obtained from $\tilde{\varrho}(r)$ within ~1-2 MeV, if also the next term after the so-called Weizsäcker term is added in the expansion of the kinetic energy density.

References.

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