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PHYSICAL REVIEW C VOLUME 2, NUMBER 5 NOVEMBER 1970

Self-Consistent Calculations of Shell Effects Including the Proposed Island of Stability*

W. H. Bassichis
Department of Physics and Laboratory for Nuclear Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 and Lawrence Radiation Laboratory, University of California, Livermore, California 94551

and

A. K. Kerman
Department of Physics and Laboratory for Nuclear Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 20 April 1970)

A study is made of the characteristics of magic nuclei displayed in a Hartree-Fock calculation. It is seen that the known doubly-closed-shell nuclei are clearly distinguished by the behavior of the energy as a function of neutron and proton number. The existence of these characteristics for the superheavy nucleus with $Z=120$ and $N=178$ indicates that this may also be a magic nucleus. Single-particle-model calculations have indicated $Z=114$ as the magic nucleus. Possible reasons for this difference are discussed.

I. EXISTENCE OF SUPERHEAVY NUCLEI

The possibility of accelerating heavy ions (e.g., Ar^{40}) has resulted in much experimental and theoretical research on an island of stability with $Z>100$. Recent experimental progress has been reviewed by Flerov.[1] Though nuclei with $Z>105$ have not as yet been formed in these experiments, the existence of such stable nuclei might be determined when it becomes possible to accelerate the heavier ions.

Theoretical calculations have been performed[2-4] which indicated that an island of stability might exist in the region of $Z=114$, $N=184$. In general, the theoretical techniques applied consist of single-particle calculations of the Nilsson type[2] combined with certain features of the liquid-drop model. Though such calculations may well provide a device for extrapolating from the known nuclei to heavier nuclei, because of their uncertainties it would also be desirable to investigate less phenomenological methods for calculating properties of superheavy nuclei.

A step in this direction has been made in the approach taken by Meldner,[5] where a degree of self-consistency has been added to the single-particle-Hamiltonian method. The technique is, essentially, to solve the single-particle equation

$$\left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}-\epsilon_\mu\right)\varphi_{\mu,\tau_t}(\vec{r})=\int d^3r' K_{\tau_z}(\vec{r},\vec{r}')\varphi_{\mu,\tau_z}(\vec{r}'), \quad (1)$$

where K, rather than being a single-particle potential directly derived from a two-body interaction, is assumed to be a nonlocal potential with a specific density dependence of the form

$$K_{\tau_z}(\vec{r},\vec{r}')=v(|\vec{r}-\vec{r}'|)\left\{1-\left[\frac{\rho_{\tau_z}(x)}{\rho_1}\right]^{2/3}\right\}\rho(x) . \quad (2)$$

Here

$$x=\tfrac{1}{2}(|\vec{r}|+|\vec{r}'|) ,$$

$$\rho_{\tau_z}=\sum_{\mu=1}^{N}|\varphi_{\mu,\tau_z}|^2 ,$$

and the nonlocality is contained in the factor v

which is taken to be a Yukawa potential with short range. After inclusion of a spin-orbit term and a term which approximates the Coulomb interaction, the equation contains five parameters. Single-particle wave functions are assumed, a density calculated, and Eq. (1) is solved. The process is repeated with the resulting wave functions until self-consistency is obtained. The resulting fit to experimental binding energies and radii of spherical nuclei near closed shells is quite good. The method was applied by Meldner to superheavy nuclei, and it was shown that $\partial E/\partial Z$ changes considerably at $Z = 114$, indicating a magic number. A significant shell effect was also found for $N = 186$.

In view of these results it is interesting to investigate the results of bona fide Hartree-Fock calculations to determine how the known magic numbers are distinguished in such a calculation and then to explore the superheavy elements for such effects.

II. HARTREE-FOCK CALCULATIONS

The first question to be faced is the choice of the nuclear force. Restricting consideration to Hamiltonians which contain only the kinetic energy and two-body interactions consistent with two-body scattering information does not unambiguously determine the Hamiltonian. Even the restriction that the two-body matrix elements of the interaction be finite leaves ambiguity, since a number of "soft" potentials have been proposed which are reasonably consistent with scattering data.[6,7]

The interaction chosen for these calculations is that of Tabakin.[6] This force is "semirealistic" in the sense that the fit to two-body data is quantitatively rather poor, and that in the long-range limit it does not have the character of a one-pion-exchange interaction. It is entirely nonlocal and acts only in relative S, P, and D states. Because of this latter property the calculation of matrix elements of the interaction is simplified and this enables one to perform rather large calculations without using a prohibitively large amount of computer time. Though the matrix elements of the Tabakin potential are quite similar to those of other realistic potentials, and to matrix elements extracted directly from scattering data,[8] the results obtained should be viewed as tentative unless it can be shown that the same results are obtained with more realistic forces.[9] It should be pointed out, however, that some of the results previously obtained with the Tabakin interaction[10,11] are quite reasonable, so that it is not necessary to consider the present calculation as *only* a demonstration of the feasibility of such a program.

In order to use the Hartree-Fock procedure to determine where shell effects appear in superheavy nuclei it is first necessary to determine how the existence of magic numbers manifests itself for the known closed shells. This could have been accomplished by using an existing computer program[12] in which single-particle wave functions were expanded in harmonic-oscillator levels belonging to the first six major shells and the $1i_{13/2}$ level. Here both radial and angular variations were allowed so that deformed, as well as spherical, nuclei could be treated. Such a space is not, however, sufficiently large to study superheavy nuclei, since it can treat no more than 126 neutrons. It was thus necessary to construct an even larger space, and this necessitated the limitation to radial variations only. Non-closed-shell nuclei can still be approximately treated by the device of a filling parameter.[13]

As is well known, the self-consistent procedure[14] consists of diagonalizing the matrix

$$\langle \alpha | h | \beta \rangle = \langle \alpha | t | \beta \rangle + \sum_{\lambda} \langle \alpha \lambda | V_A | \beta \lambda \rangle , \tag{3}$$

where t is the kinetic-energy operator, V_A the antisymmetrized two-body interaction, $|\alpha\rangle$ and $|\beta\rangle$ are states in an arbitrary representation (taken here

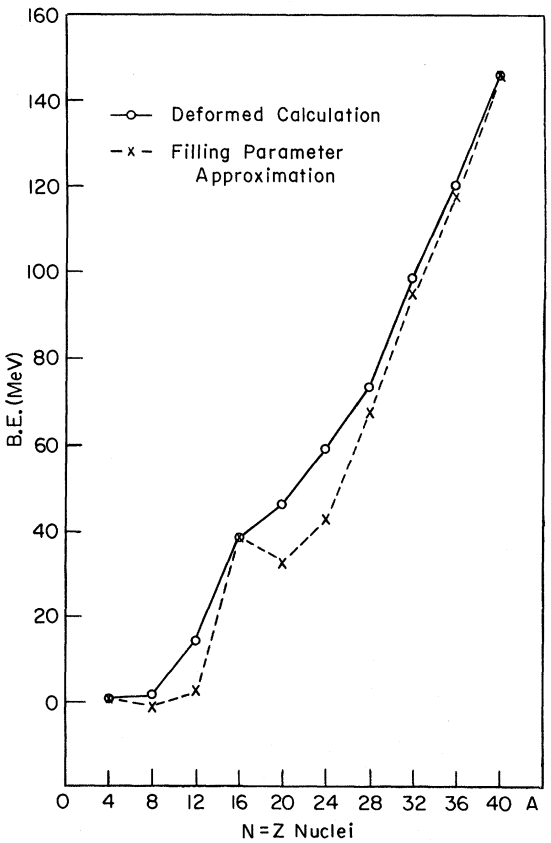

FIG. 1. Comparison of the binding energies obtained using a filling-parameter approximation and a deformed calculation. The largest errors occur for the nuclei with the largest deformation.

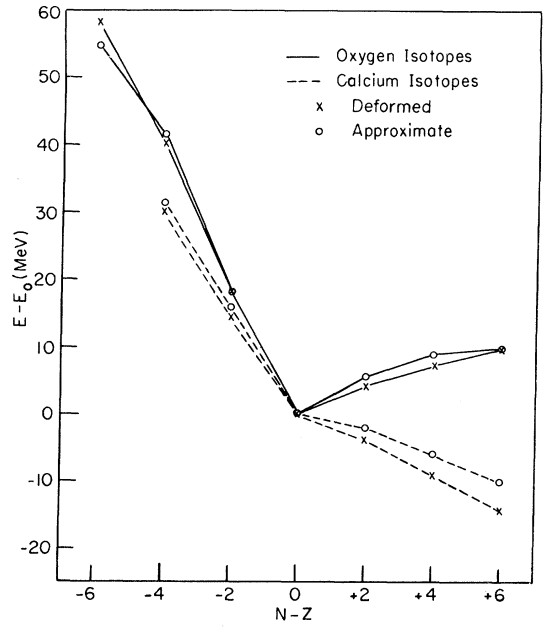

FIG. 2. Comparison of the binding energies obtained with and without the filling-parameter approximation for nuclei near a closed shell.

to be harmonic oscillators), and $|\lambda\rangle$ are the occupied states which are determined self-consistently. Under the assumption of spherical symmetry, sums over Clebsch-Gordan coefficients can be performed, so that the matrix equation becomes

$$\langle\alpha|h|\beta\rangle_\tau = \langle\alpha|t|\beta\rangle_\tau + \sum_{\lambda\tau_\lambda}\sum_{ij}\sum_{JT}\frac{(2J+1)}{(2j_\alpha+1)} \times\langle\tfrac{1}{2}\tau\tfrac{1}{2}\tau_\lambda|T,\tau+\tau_\lambda\rangle^2\langle\alpha i|V_A|\beta j\rangle_{JT}C_i^{\lambda\tau\lambda}C_j^{\lambda\tau\lambda}. \quad (4)$$

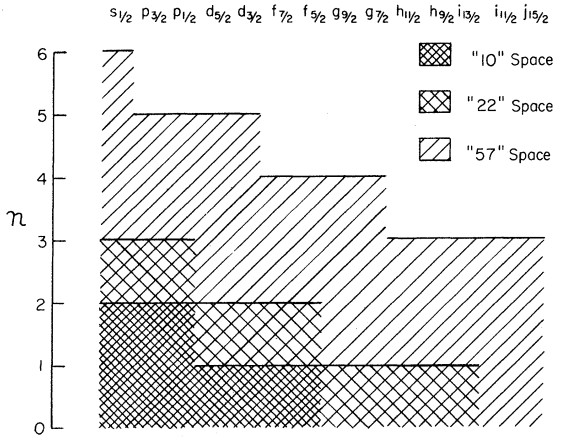

FIG. 3. The harmonic-oscillator bases used in various calculations, where n is the principal quantum number.

Here the C's are the expansion coefficients and the states α, β, i, j, and λ are characterized only by n, l, and j rather than by n, l, j, m, and τ_z, and the matrix element is now coupled to good total isospin T and angular momentum J. As mentioned above, the treatment can be modified for non-closed-shell nuclei by modifying the factor

$$\frac{2J+1}{2j_\alpha+1} = \frac{2J+1}{(2j_\alpha+1)(2j_\lambda+1)}(2j_\lambda+1) \quad (5)$$

to

$$\frac{2J+1}{(2j_\alpha+1)(2j_\lambda+1)}\theta(\lambda),$$

where $\theta(\lambda)$, the filling parameter, is the actual number of particles in a particular λ level instead of the maximum number, $2j_\lambda+1$.

Before going on to the consideration of shell effects, it is necessary to determine the accuracy of the filling-parameter approximation. A comparison of the results thus obtained with those of a calculation in a space containing the same number of shells but allowing for deformations is given in Fig. 1. These calculations were carried out using as a basis the harmonic-oscillator eigenfunctions

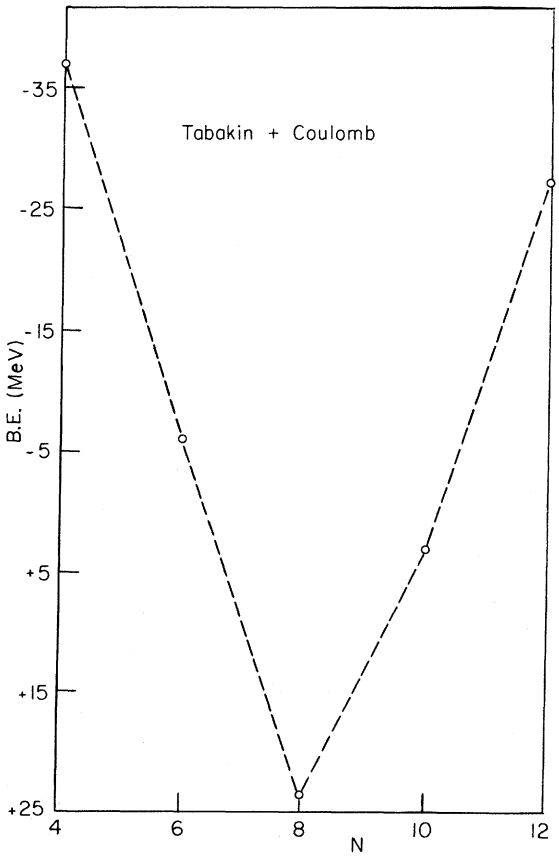

FIG. 4. The calculated energies of the $A=16$ nuclei as a function of neutron number.

of the first six major shells plus the $1i_{13/2}$. It is to be noted that the largest deviations naturally occur for those nuclei which are most strongly deformed. Since the regions of primary interest are those near the spherical region, it is more relevant to consider the results for nuclei near O^{16} and Ca^{40} This comparison is made in Fig. 2. The conclusion is that in the neighborhood of the spherical nuclei, where deformations are expected to be small, the filling-parameter approximation is valid.

Calculations were then carried out in a much larger space which would allow radial variations even for the high j levels being filled in superheavy nuclei. The size of the basis utilized is shown in Fig. 3, where it is labeled 57, corresponding to the number of n,l,j levels it contains. The 22 and 10 spaces, used previously to study truncation effects,[12] are shown for comparison.

III. SHELL EFFECTS IN OXYGEN, CALCIUM, AND LEAD

Though empirically the characteristics of nuclei with a magic number of protons and neutrons are

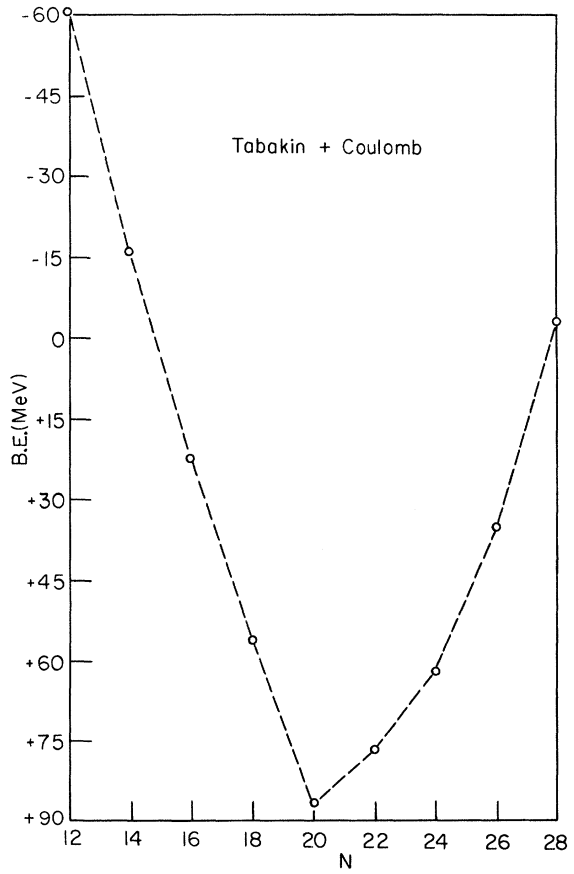

FIG. 5. The calculated energies of the $A=40$ nuclei as a function of neutron number.

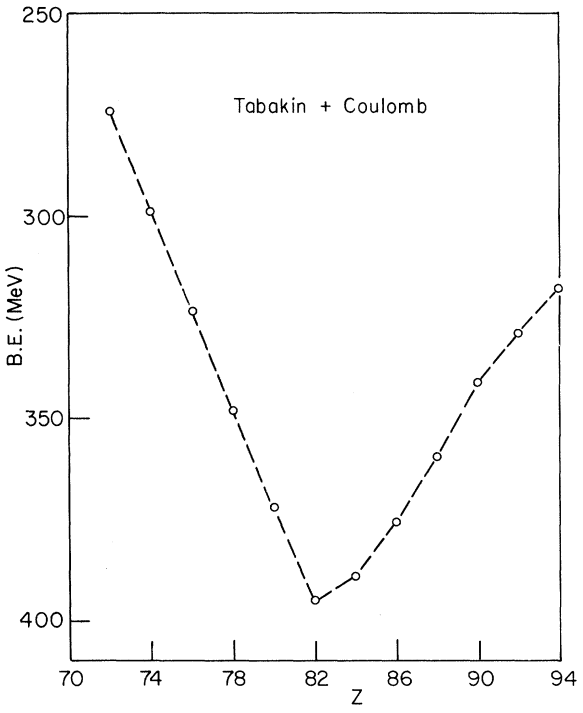

FIG. 6. The calculated energies of the $A=208$ nuclei as a function of proton number.

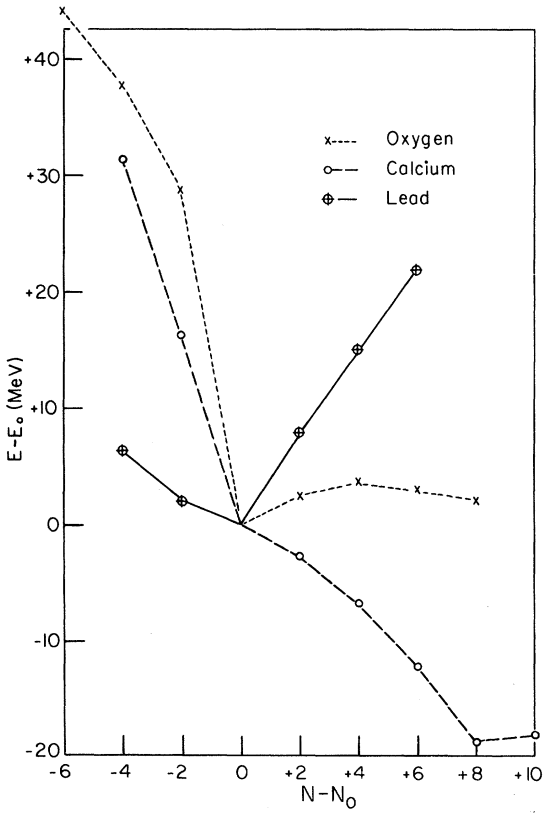

FIG. 7. The calculated difference in energy between isotopes and the appropriate magic nucleus.

well known, it is not clear which of these properties, if any, would emerge from a Hartree-Fock calculation. The obvious calculation of binding energies and separation energies might be expected to show the shell structure. But the use of a determinantal wave function cannot lead to both calculated binding energies and separation energies which agree with experiment.[7] In fact, results using "realistic" potentials are not in quantitative agreement with either experimental quantity.[12] Though at least qualitative agreement can be obtained using a perturbation expansion,[10] such a program has not yet been carried out for heavy nuclei. A possible criterion for magic nuclei in a Hartree-Fock framework might be the existence of an unusually large gap between the occupied and unoccupied orbits. Such a test is complicated if the filling-parameter approximation is employed. We therefore examine the variation in the binding energy as a function of neutron and/or proton number to look for characteristic behavior at magic numbers, even though the absolute magnitude of the quantity itself is far from the experimental value.[4] That this is indeed the case can be seen in Figs. 4–8.

Figures 4 and 5 show the behavior of the binding energy of the $A = 16$ and $A = 40$ systems as a function of neutron number. The Coulomb interaction has been included self-consistently. The result that the most stable nucleus has $N = Z$ is not surprising, since this is a symmetry effect. The results shown in Fig. 6 for the $A = 208$ system are, however, more significant. There it is seen that, despite all the deficiencies of the two-body interaction employed, and the inherent limitations of the Hartree-Fock method, the calculation is consistent with the experimental shell effect at $N = 126$, $Z = 82$. This implies that the balance between Coulomb and symmetry effects is roughly correct.

The shell effect manifests itself directly in dE/dZ and dE/dN. In Fig. 7 are plotted the binding energies of the oxygen, calcium, and lead isotopes as a function of neutron number, where N_0 is the magic number of neutrons appropriate for each element. The characteristic feature of magic numbers is present, that is, a sharp decrease in the energy gained by adding neutrons at the magic number. In fact, this effect is exaggerated by the calculation to such an extent that for oxygen and lead the energy gained by adding neutrons beyond the magic number becomes negative, indicating, for

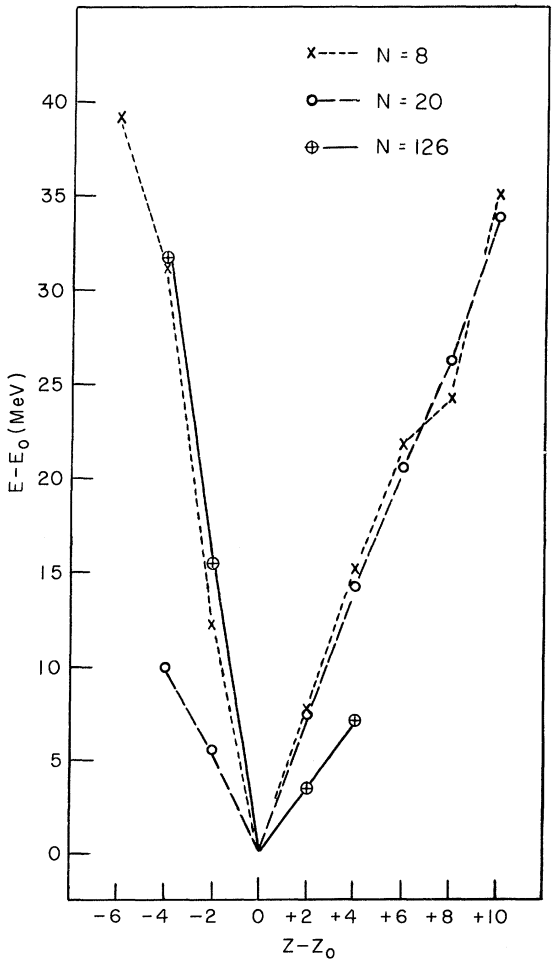

FIG. 8. The calculated difference in energy between isotones and the appropriate magic nucleus.

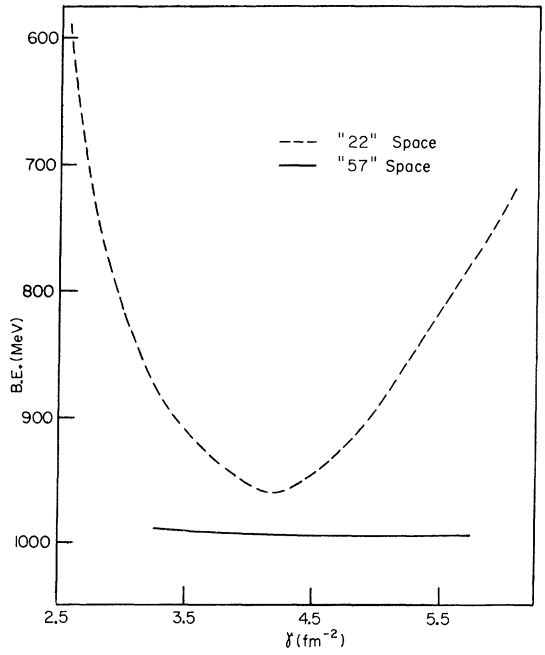

FIG. 9. The variation in the calculated binding energy of Pb^{208} with the oscillator parameter γ when only the nuclear force is considered.

example, that O^{18} is less bound than O^{16}. This effect is not a result of the θ approximation, as can be deduced from Fig. 2. In fact, second-order calculations of the energy do tend to correct this discrepancy,[10,11] leaving the shell effect. This exaggeration is actually useful, since it magnifies the effect which will be searched for in the superheavy region.

In Fig. 8 are shown the $N=8$, 20, and 126 isotones as a function of proton number, where Z_0 is the appropriate magic number of protons. Here again the characteristic behavior of the binding energy in the neighborhood of doubly-closed-shell nuclei is evident and again exaggerated by the calculation.

The above calculations were carried out in the "57" space consisting of nearly 11 major shells (see Fig. 3), and the Coulomb force was used in addition to the Tabakin interaction. Though the space employed was so large that little dependence on the oscillator parameter γ was expected, all calculations were carried out using the optimum γ for each nucleus. This will be discussed further in the next section.

IV. APPLICATION TO SUPERHEAVY NUCLEI

The results given in the previous section indicate that the Hartree-Fock procedure can indeed be used to try to locate magic numbers in superheavy nuclei. It first must be ascertained whether or not the space (in which the single-particle levels are being expanded) is large enough for large numbers of particles. One method of determining the degree to which the space may be considered complete is to examine the dependence of the results on γ. If there is a dependence, then variations with respect to this parameter must be carried out, and only results at the optimum γ are meaningful. Figure 9 shows the variation of the calculated binding energy of Pb^{208} with γ in the "22" and "57" spaces of Fig. 3. These calculations were done without the Coulomb force. The independence of the energy in the "57" space leads to the conclusion that the space is essentially complete for at least 126 particles (either protons or neutrons), and the same calculation for a superheavy nucleus, $Z=114$, $N=184$, showed a similar independence of the energy to variation in γ.

This independence is to a small extent destroyed when the Coulomb force is included in the calculations. The variation of the energies of Pb^{208} and the $Z=114$, $N=184$ nucleus with γ when the Coulomb force is included self-consistently is shown in Fig. 10. It should be pointed out that for a wide range of γ's in the neighborhood of the optimum value the energy is quite independent of γ, indicating that the space is sufficiently large. However, as will be shown later, erroneous conclusions can be drawn from calculations employing a γ far from the optimum value, because of the dependence introduced by addition of the Coulomb force.

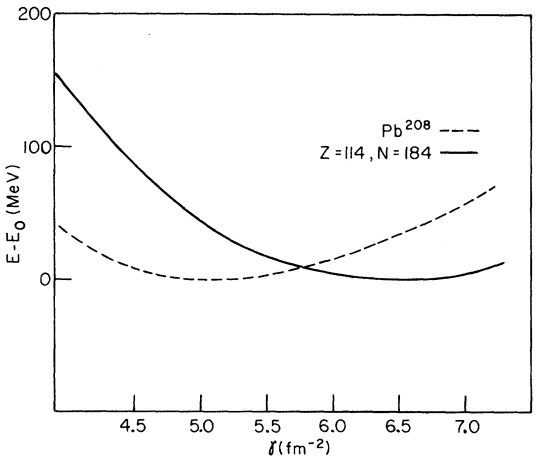

FIG. 10. The variation in the calculated binding energies of Pb^{208} and the $Z=114$, $N=184$ nucleus in the 57 space with γ when the Coulomb is force included.

The results of Meldner[5] lead to consideration of the nuclei with mass number 298. The calculated binding energies of these nuclei as a function of proton number is given in Fig. 11. The results

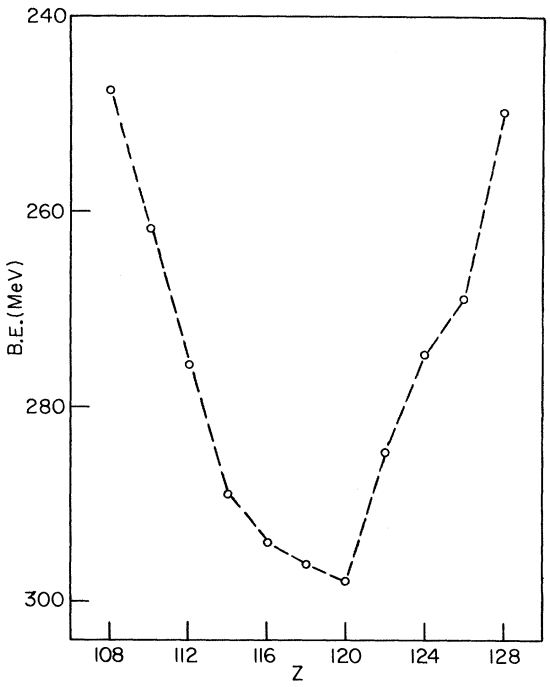

FIG. 11. The calculated energies of the $A=298$ nuclei as a function of proton number.

were obtained using the optimum γ for these nuclei. Clearly the indication of these calculations is that the most likely candidate for designation as a magic number is $Z = 120$. This is strongly reinforced by the results shown in Fig. 12, a graph of the binding energy as a function of Z for fixed N. For both values of N shown there is no evidence for a shell closure at $Z = 114$, while at $Z = 120$ the sharp change in $\partial E/\partial Z$, characteristic of the known magic proton numbers (see Fig. 8), is again striking. The designation of a neutron number as magic is less clear. The variation of the binding energy for fixed Z as a function of N is shown in Fig. 13. Apparently both $N = 178$ and $N = 184$ are candidates for the designation.

The existence and location of sharp changes in binding energy as a function of neutron or proton number depends strongly on the corresponding single-particle energies. For example, in the single-particle model of Nilsson[2] it is the large spin-orbit splitting of the $2f$ orbit in the proton spectrum that leads to a large change in $\partial E/\partial Z$ at $Z = 114$, where the $2f_{7/2}$ is filled and the $2f_{5/2}$ is empty. This splitting results from a particular set of parameters in the single-particle Hamiltonian, which were fitted to observed quantities for lighter nuclei and extrapolated to the superheavy region. A similar extrapolation procedure was also employed in the calculation of Meldner.[5] In the Nilsson (or Rost[15]) spectrum for Pb^{208} there is a spin-orbit splitting of about 4 MeV for the $2f$ levels. Using extrapolated parameters for the $A = 290$ region ($Z \approx 114$), this splitting was only slightly reduced and a large single-particle gap remained.

The question of single-particle energies is rather different in the Hartree-Fock framework. Given the two-body interaction, there are no adjustable parameters and the single-particle energies are the eigenvalues of the self-consistent Hamiltonian, which of course depends on the number of particles in the system. There is, therefore, no external extrapolation procedure involved. Furthermore, the significance of the Hartree-Fock spectrum is quite different from that of a single-particle model. The self-consistent single-particle energies which emerge from a Hartree-Fock calculation can be compared with observed separa-

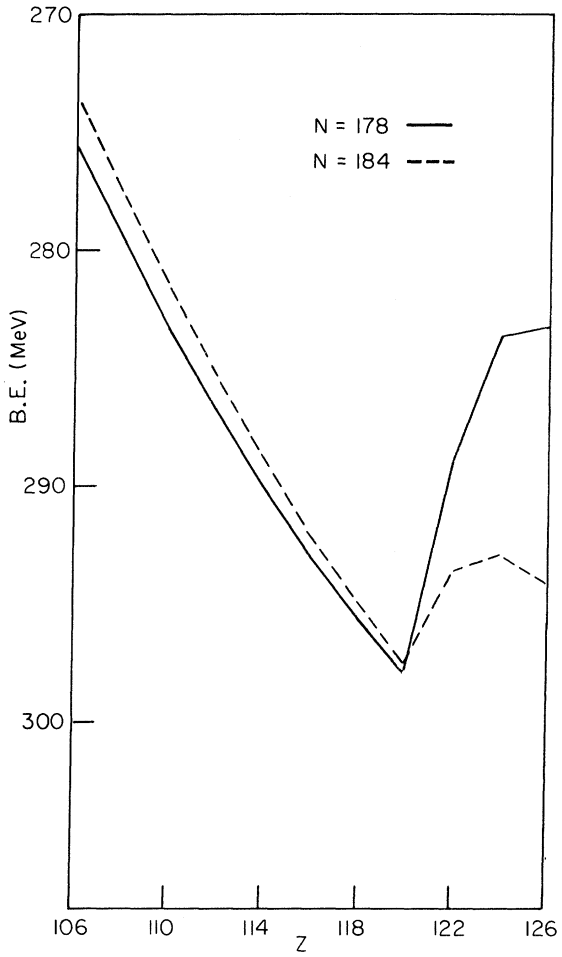

FIG. 12. The calculated energies of the $N = 178$ and $N = 184$ isotones as a function of proton number.

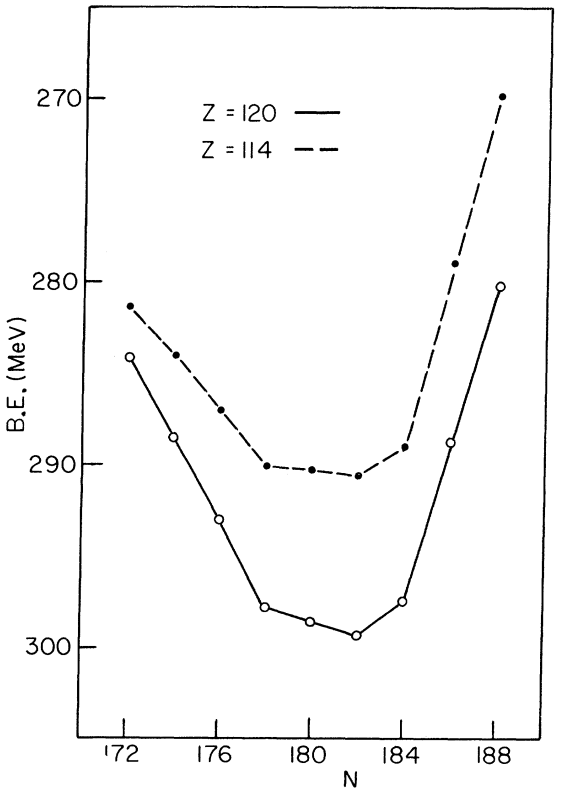

FIG. 13. The calculated binding energies of the $Z = 114$ and $Z = 120$ isotopes as a function of neutron number.

tion energies only after two corrections have been effected. The orbital-rearrangement correction involves the change in the Hartree-Fock potential, and the subsequent change in the energy, when the $A-1$-particle system, rather than the A-particle system, is treated self-consistently. This correction is rather small,[10] even in light nuclei, and should decrease in magnitude as A increases. The difference between $E_{\mathrm{HF}}(A)$ and $E_{\mathrm{HF}}(A-1)$ still cannot be compared with experimental separation energies, because each energy is only to be considered as the first term in a perturbation calculation. The second-order terms in the perturbation expansion take into account two-particle correlations, which are different in the A and $A-1$ systems. Approximate calculations of these second-order terms[10] have shown that the correlation corrections are significantly different for the A- and $A-1$-particle systems and, furthermore, are dependent on the particular state of the hole in the $A-1$ system.

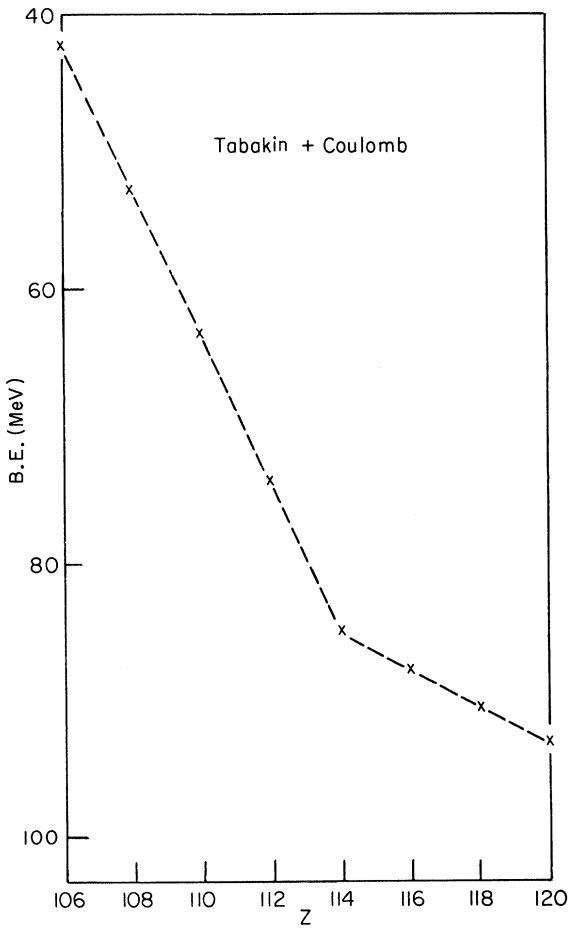

FIG. 14. The calculated binding energies of the $N=184$ isotones as a function of proton number when the value of the oscillator parameter is far from the optimum value.

In view of the above remarks, it is rather a coincidence that the Hartree-Fock spectrum for Pb^{208} exhibits a spin-orbit splitting of about 4 MeV in the first unoccupied f levels, as in the Nilsson model. In contrast to this there is a change in the self-consistent Hamiltonian, resulting from the addition of particles to the system, which leads to a reduction in this splitting to about 1.5 MeV for the superheavy region.

The Hartree-Fock and Nilsson spectra for the $A=290$ region differ also in the position of the $i_{13/2}$ level relative to the f levels. While both spectra show the $i_{13/2}$ level losing binding relative to the f levels as A increases from 208 to 290, this level is still more bound than the $2f_{5/2}$ in the Nilsson picture at $A=290$, and slightly less bound than the second $f_{5/2}$ level in the Hartree-Fock spectrum. Thus in the Hartree-Fock picture, the second $f_{7/2}$ and $f_{5/2}$ orbits are filled when $Z=106$. Since the gap between the $f_{5/2}$ and $i_{13/2}$ levels is small, there is no shell effect there. Between $Z=106$ and 120, the $i_{13/2}$ level becomes filled, so that $\partial E/\partial Z$ is smooth in this region. In the self-consistent single-particle spectrum for $Z=120$ there is a considerable gap between the highest occupied state (first $i_{13/2}$) and the lowest unoccupied state (third $p_{3/2}$). The resulting discontinuity in $\partial E/\partial Z$ is shown in Fig. 12. It was found that even if the $i_{13/2}$ level were filled before the second f levels, the absence of a gap between the $f_{7/2}$ and $f_{5/2}$ levels and the existence of a gap between the third $p_{3/2}$ and the occupied levels leads to the discontinuity in $\partial E/\partial Z$ at $Z=120$ rather than at $Z=114$.

All of the above conclusions follow from calculations in which the optimum γ (6.7 fm^2) was employed for this range of A. As can be deduced from Fig. 10 (and was verified by calculation), the same results obtain for a range of values for γ in the neighborhood of the optimum value. Preliminary calculations[16] were made with a value far from the optimum (3.7 fm^2), and the results obtained for the energy as a function of Z are shown in Fig. 14. The discontinuity in $\partial E/\partial Z$ at $Z=114$ with this inappropriate γ stems from a single-particle spectrum quite similar to Nilsson's[2] which, as was pointed out, changes rather dramatically when the correct value is utilized. The possibility of obtaining misleading results when an inappropriate γ is used has been previously pointed out.[17]

V. CONCLUSION

It has been shown that the magic numbers 8, 20, 82, and 126 can be identified by discontinuities in $\partial E/\partial Z$ or $\partial E/\partial N$ and minima in $E(N-Z)$ for constant A when the energy has been calculated in the

Hartree-Fock approximation. Utilization of a very large number of basis states has made possible an extension of the calculations to the superheavy region where 120 appears as a magic proton number, and either 178 or 184 as a magic neutron number. Since the "realistic" force employed is known to have certain deficiencies, it will be interesting to repeat these calculations with other two-body interactions to see if the discrepancy between predictions based on self-consistent calculations and those which rely on phenomenological single-particle Hamiltonians persists.

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*Work supported in part through funds provided by the U. S. Atomic Energy Commission under Contract No. AT (30-1) 2098.

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