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Nilsson-like single particle model

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An independent particle model is obtained from the fundamental constrained variational equations for a many-body system by making certain assumptions. The resulting model contains the attractive feature of the Nilsson model but has the advantage of a traceable connection to the exact equations and thus is more amenable to interpretation. In particular, the energy deformation surface is calculated using the new model and is shown to differ significantly from the one obtained in the usual approach.

[NUCLEAR STRUCTURE Modified independent particle model proposed and compared to that of Nilsson.]

I. INTRODUCTION

The independent particle model of Nilsson[1] has been widely used in almost all branches of nuclear physics. Although the model is extraordinarily simple, it predicts the correct spins and parities for most ground states and low-lying excited states and gives reasonable agreement with experimental electromagnetic transition rates, etc., when combined with a collective model.[2] Recently there has been renewed interest in the model because of the Strutinsky ansatz,[3] through which one may combine the macroscopic liquid drop model and the microscopic independent particle model.[4]

In addition to using the Nilsson model there has been considerable interest in testing the model within the framework of a more fundamental theory, such as constrained Hartree-Fock.[5] These investigations have pointed out certain theoretical deficiencies primarily related to the popular prescription for obtaining the ground state deformation.

Because of its theoretical weaknesses and the fact that there are instances where the present Nilsson model does not lead to reasonable agreement with experiment, a modified model is presented here. This model has its basis in theory so that the previous difficulties can be eliminated. By construction, the main virtues of the Nilsson model are retained but there are differences in the results of the two models. The differences are just of the sort that would have a large effect on Strutinsky calculations.

In order to establish notation, the next section contains a brief summary of the method of constrained Hartree-Fock (CHF). This is followed by the usual development of the Nilsson model, and the difficulty of drawing a correspondence with CHF is demonstrated. Finally the new model is developed and the results of the two models compared for typical nuclei.

II. CONSTRAINED HARTREE-FOCK

The usual Hartree-Fock method consists of using the variational method on the set of wave functions consisting of all determinants of single particle states. Thus, if

$$\Phi = \prod_{i=1}^{A} a_\lambda^\dagger |0\rangle$$

is the "best" determinant, it satisfies the equation

$$\delta E = \delta\langle\Phi|H|\Phi\rangle = 0 ,$$

where

$$H = \sum_{\alpha\beta} \langle\alpha|t|\beta\rangle a_\alpha^\dagger a_\beta + \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|V|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma .$$

Here α,β can be any representation and the single particle states λ satisfy the equation

$$(h-\epsilon_\lambda)|\lambda\rangle = 0$$

or, in the α,β representation,

$$\langle\alpha|h|\beta\rangle\langle\beta|\lambda\rangle = \epsilon_\lambda\langle\alpha|\lambda\rangle .$$

The matrix h is called the Hartree-Fock matrix and is given by

$$\langle\alpha|h|\beta\rangle = \langle\alpha|t|\beta\rangle + \sum_\lambda \langle\alpha\lambda|V_A|\beta\lambda\rangle$$
$$= \langle\alpha|t|\beta\rangle + \langle\alpha|U|\beta\rangle .$$

The energy

$$E = \sum_\lambda \langle\lambda|t|\lambda\rangle + \tfrac{1}{2}\sum_{\lambda\mu}\langle\lambda\mu|V_A|\lambda\mu\rangle$$

and the "single particle energies" ϵ_λ are related via

$$E=\tfrac{1}{2}\sum_{\lambda}(\epsilon_{\lambda}+\langle\lambda|t|\lambda\rangle).$$

Since the Hartree-Fock potential U depends on the solutions to the problem, λ, the equations must be solved by iteration. It is important to note that this potential is nonlocal and, except for special situations, not spherically symmetric. It should be emphasized that the diagonalization of the Hartree-Fock matrix is *equivalent* to minimization of E only if h, and not some approximation to it, is the matrix diagonalized.

Solving these equations will yield a number of solutions, depending on the starting guess for the λ's. In ^{12}C, for example, guessing a spherically symmetric determinant will lead to a spherically symmetric solution. An oblate solution and a prolate solution can also be obtained with the appropriately deformed initial wave functions. If, instead, one wishes to map out the entire energy surface, then constraints must be included using, for example, the method of Lagrange multipliers. Instead of minimizing the expectation value of H, it is the expectation value of $H-\Lambda Q$ which must be minimized, where Λ is the Lagrange multiplier and Q is the operator whose expectation value is to be constrained. There may be many such operators, each with its corresponding Λ, but for simplicity only one, the quadrupole moment $\sum_i q_i$, will be considered here.

The single particle matrix which must now be diagonalized is

$$\langle\alpha|\tilde{h}|\beta\rangle=\langle\alpha|t|\beta\rangle+\langle\alpha|U|\beta\rangle-\Lambda\langle\alpha|q|\beta\rangle,$$

where Λ is a constant for each calculation. Since it is

$$\mathcal{E}=\langle H-\Lambda Q\rangle=E-\Lambda\langle Q\rangle$$

which is minimized, one has

$$\frac{d\mathcal{E}}{dQ}=0=\frac{dE}{dQ}-\Lambda$$

so that the Lagrange multiplier is related to the derivative of the energy and, naturally, the minima in $E(Q)$ correspond to $\Lambda=0$. Furthermore, the relationship between the single particle energies and the total energy must be corrected for the presence of the constraint in $\tilde{h}$. Thus, when constraints are added,

$$E=\tfrac{1}{2}\sum_{\lambda}(\tilde{\epsilon}_{\lambda}+\langle\lambda|t|\lambda\rangle-\Lambda\langle\lambda|q|\lambda\rangle).$$

III. THE NILSSON MODEL

In the independent particle model of Nilsson one considers the deformed harmonic oscillator potential with an $\vec{l}\cdot\vec{s}$ and an $\vec{l}^2$ term added to it:

$$h_N=\frac{-\hbar^2}{2m}\nabla^2+\tfrac{1}{2}m(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2)+C\vec{l}\cdot\vec{s}+D\vec{l}\cdot\vec{l}.$$

The potential normally considered is axially symmetric so that

$$\omega_x=\omega_y$$

and the usual parametrization of these oscillator parameters is in terms of δ and ω:

$$\omega_x^2=\omega_y^2=\omega^2(1+\tfrac{2}{3}\delta),\quad \omega_z^2=\omega^2(1-\tfrac{4}{3}\delta).$$

The frequency ω is then made a function of the deformation because of the assertion that the nuclear volume must be a constant. This follows from the postulate of nuclear incompressibility. Thus one sets

$$\omega_x\omega_y\omega_z=\text{constant}$$

so that

$$\omega=\omega(\delta)=\omega_0(1-\tfrac{4}{3}\delta^2-\tfrac{16}{27}\delta^3)^{-1/6}.$$

One then diagonalizes the Nilsson single particle Hamiltonian,

$$h_N=t+\tfrac{1}{2}m\omega^2r^2+\delta m\omega^2r^2Y_{20}+C\vec{l}\cdot\vec{s}+D\vec{l}\cdot\vec{l}$$
$$=t+U_0+\delta\gamma q,$$

and obtains the Nilsson single particle energies $\epsilon(\delta)$. The parameters ω, C, and D are adjusted to reproduce the single particle spectrum for the spherical nuclei. The prescription for calculating the equilibrium deformation for a nucleus with A particles is to sum the lowest A eigenvalues ϵ as a function of δ and minimize.

IV. CORRESPONDENCE WITH CHF

It is quite tempting to consider the Nilsson model to be an approximation to constrained Hartree-Fock. In particular, one may write the CHF potential as a spherical part plus a deformed part, assumed to be of a quadrupole character,

$$U_{\mathrm{CHF}}=U_s+\xi q.$$

Then the CHF one body Hamiltonian

$$h=t+U_s+\xi q-\Lambda q=t+U_s+(\xi-\Lambda)q$$

and the Nilsson Hamiltonian

$$h=t+U_0+\delta\gamma q$$

are, indeed, of the same form.

From this point of view the main difficulty with the Nilsson model would be the inability to separate the Nilsson deformation parameter δ into its two components: ξ representing the deformed potential generated by the single paraticle wave

functions and Λ, the external constraint. Without such a separation one cannot compensate for the presence of the constraint in the Hamiltonian generating the ϵ's and thus cannot calculate the energy. Thus one must use some prescription, such as the summation of the ϵ's, and these have been tested and found to be unsatisfactory,[6] both for determining equilibrium deformations and for reproducing the fluctuations in the energy, as needed in the Strutinsky procedure.

There are other difficulties with the Nilsson model in addition to those associated with the Lagrange multiplier. The idea of constant nuclear volume is, at best, imprecise. It would be preferable, therefore, if the results were not particularly sensitive to the form of the functional dependence of ω on δ. However, if one performs Nilsson calculations with

$$\omega(\delta) = \omega_0(1 - \alpha\tfrac{4}{3}\delta^2 - \alpha\tfrac{16}{27}\delta^3)^{-1/6}$$

instead of the usual form $\alpha = 1$, it is found that the location of the minima in $\epsilon(\delta)$, for example, is quite sensitive to the value of α. This is shown in Fig. 1 where the sum of the single particle energies is shown as a function of δ with α having different values. Furthermore, the property that the density of the nucleus should not be a function of deformation, or not depend strongly on it, should be expected to come out of a calculation and not be an input to it.

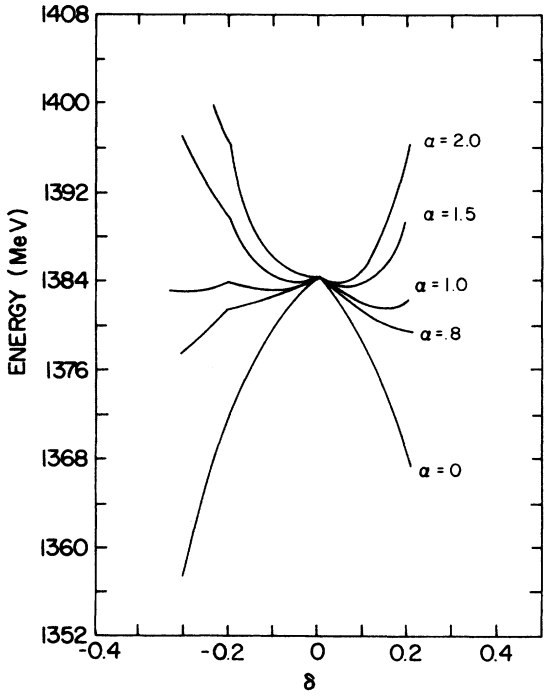

FIG. 1. Family of curves of $\Sigma\epsilon$ versus δ for 44 particles with α as the parameter. The curves illustrate the strong dependence of the energy surface on the precise formulation of volume conservation.

V. A MODIFIED INDEPENDENT PARTICLE MODEL

In this section a model will be developed which retains the advantages of the Nilsson model but has the Lagrange multiplier appearing explicitly and, to some extent, eliminates the need for imposing the constant volume condition.

In order to reproduce the fit to single particle spectra at equilibrium deformations the model is required to predict the same equilibrium deformations. This implies that the deformations at which $\Sigma\epsilon$ has minima are to be characterized by $\Lambda = 0$ in a constrained variational calculation or that, at these points, the single particle potential has been generated only by the single particle wave functions. This requirement alone is not consistent with the identification of the Nilsson Hamiltonian with the CHF Hamiltonian. One may, for example, attempt to incorporate this requirement into the Nilsson model by writing

$$h_N = t + U_0 + \delta_{\min} q + (\delta - \delta_{\min})q\,,$$

where the constant γ has been set equal to one and where $\delta_{\min}$ characterizes a deformation at which $\Sigma\epsilon$ has a minimum. Since it has been demonstrated that the total CHF energy is well approximated, in the region of a minimum, by keeping the nuclear potential fixed and varying only the Lagrange multiplier, it is reasonable to identify the fixed potential $U_0 + \delta_{\min} q$ as the nuclear potential and $(\delta - \delta_{\min})$ as the Lagrange multiplier.[7] Having thus identified Λ one can "properly" calculate the energy as a function of deformation via

$$E(\bar{Q}) = \langle T\rangle + \langle V\rangle$$
$$\approx \tfrac{1}{2}\sum_\lambda (\epsilon_\lambda + \langle\lambda|t|\lambda\rangle - \Lambda\bar{Q})\,,$$

where

$$\bar{Q} = \sum_\lambda \langle\lambda|q|\lambda\rangle\,.$$

This energy is approximate because the ϵ_λ are not the eigenvalues of the matrix that results from minimizing $H - \Lambda Q$ but rather of a matrix in which the nonlocal, self-consistent potential has been replaced by the local harmonic oscillator potential. But because the relationship between E and ϵ_λ is now not exact, the approximate expression for $E(\bar{Q})$ does not satisfy the condition that

$$\frac{dE}{d\bar{Q}} = -\Lambda$$

and, more specifically, the minimum in $E(\bar{Q})$ does

not correspond to the deformation δ_{min}. Thus one has an inconsistency. The points δ_{min} are supposed to correspond to the deformations at which there is not a Lagrange multiplier. The energy $E(Q)$ is not, however, a minimum at these points. Numerically the shifts in the minima are large so that the inconsistency is practical as well as theoretical.

The inconsistency can only be removed if the quantity being minimized and the single particle matrix being diagonalized are in *exact* correspondence. Thus, instead of minimizing the exact expectation value of a Hamiltonian and then approximating the potential part of the resulting one body Hamiltonian, one should approximate before minimizing. The approximate energy and the resulting one-body Hamiltonian would then have the correct correspondence, and relations between E and the ϵ's could be retained.

One thus begins with the expectation value of the Hamiltonian, in a determinantal wave function,

$$\langle H\rangle = \langle T+V\rangle$$

$$= \sum_{\lambda} \langle \lambda | t | \lambda\rangle + \tfrac{1}{2}\sum_{\lambda\mu} \langle \lambda\mu | V_A | \lambda\mu\rangle$$

$$= \sum_{\lambda} \langle \lambda | t+U | \lambda\rangle .$$

Here U is the nonlocal potential given, in coordinate space, by

$$U(\vec{r},\vec{r}\,') = \sum_{\mu}\left[\int d^3r_1 \int d^3r_2 \psi_\mu^*(\vec{r}_1)\langle \vec{r}\vec{r}_1 | V | \vec{r}\,'\vec{r}_2\rangle \psi_\mu(\vec{r}_2) - \int d^3r_1 \int d^3r_2 \psi_\mu^*(\vec{r}_1)\langle \vec{r}\,\vec{r}_1 | V | \vec{r}_2\vec{r}\,'\rangle \psi_\mu(\vec{r}_2)\right]$$

for a general, nonlocal, two-body interaction V. It is a rather extreme approximation to replace this complicated, wave-function-dependent operator by a deformed harmonic oscillator potential, but that is essentially what is done in the usual Nilsson model. There, however, the replacement is made after minimization of $\langle H\rangle$ with respect to the single particle states $|\lambda\rangle$, i.e., in the single particle Hamiltonian. Here the approximation will be made in the expression for the energy itself. Thus, calling the local deformed oscillator potential $U(\delta_{min})$ one writes

$$\langle H\rangle \approx \sum_{\lambda} [\langle \lambda | t | \lambda\rangle + \langle \lambda | U(\delta_{min}) | \lambda\rangle] = \langle \tilde{H}\rangle ,$$

where δ_{min} is used to characterize the deformation at the minimum.

If one wishes to obtain an energy-deformation surface then, of course, a single calculation will not suffice. Instead one may use the method of Lagrange multipliers and minimize, instead of $\langle \tilde{H}\rangle$, the expectation value of a constrained Hamiltonian

$$\mathcal{H} = \tilde{H} + \Lambda Q .$$

Then, keeping $U(\delta)$ fixed in accordance with the aforementioned approximation,

$$\langle \mathcal{H}\rangle = \sum_{\lambda} [\langle \lambda | t | \lambda\rangle + \langle \lambda | U(\delta_{min}) | \lambda\rangle + \Lambda\langle \lambda | q | \lambda\rangle]$$

is to be minimized for all values of Λ. This is equivalent to diagonalizing the one-body matrix

$$\langle i | h | j\rangle = \langle i | t | j\rangle + \langle i | U(\delta_{min}) | j\rangle + \Lambda\langle i | q | j\rangle$$

for all values of Λ. The (approximate) energy E is related to the eigenvalues of h via

$$E = \sum_{\lambda} (\epsilon_\lambda - \Lambda\langle \lambda | q | \lambda\rangle) .$$

Since the sum of the eigenvalues,

$$\sum_{\lambda} \epsilon_\lambda \equiv \mathcal{E} ,$$

is the quantity minimized for each Λ, $\partial\mathcal{E}/\partial Q$ is everywhere zero. Thus

$$\frac{\partial E}{\partial Q} = -\Lambda$$

and the minimum in the "energy" does indeed correspond to no Lagrange multiplier. To complete the model one writes

$$\Lambda = \gamma(\delta - \delta_{min})$$

thus defining a new deformation parameter δ. The single particle Hamiltonian to be diagonalized then has the form

$$\langle i | h | j\rangle = \langle i | t | j\rangle + \langle i | U(\delta_{min}) | j\rangle + \gamma(\delta - \delta_{min})\langle i | q | j\rangle$$

and since, by hypothesis

$$U(\delta_{min}) = \gamma\delta_{min} q + U_0 ,$$

this becomes

$$\langle i|h|j\rangle = \langle i|t|j\rangle + \langle i|U_0|j\rangle + \delta\gamma\langle i|q|j\rangle .$$

This is just the original Nilsson Hamiltonian. The resulting energy-deformation surface is *not*, however, the same as that obtained in a Nilsson calculation. Here one knows the Lagrange multiplier and can thus *calculate* the (approximate) energy and does not have to rely on an ansatz that has proven incompatible with theory.

VI. RESULTS

In order to calculate the energy of a nucleus as a function of deformation, one first performs the usual Nilsson calculations. This includes the determination of the free parameters so that, for the nucleus in question, the fit to the ground state deformation and the single particle spectrum at that deformation is optimized. Volume conservation is imposed as an integral part of the parameter determination. The ground state deformation is associated with the minimum in the function $\Sigma\epsilon(\delta)$.

For each configuration, the internal part of the one-body potential is then assumed to have the fixed deformation $\delta = \delta_{\min}$. The condition of volume conservation is then dropped with, instead, ω being given by $\omega(\delta_{\min})$. The energy as a function of δ is then calculated from

$$\tilde{E}(\delta) = \Sigma_\lambda \epsilon_\lambda + \Lambda\langle Q\rangle .$$

The comparison of $\tilde{E}(\delta)$ and the usual Nilsson energy surface for systems containing 42, 44, 54, 56, and 64 particles is shown in Figs. 2 through 6. These particular systems were chosen because they contain enough particles so that the energy surface has a degree of structure but, few enough so that the computing time is still small for any calculation. In each graph the solid curve is the result of the modified calculation and the dotted curve is the usual Nilsson result. First, it is clear that the "equilibrium deformations" or minima in the energy surfaces coincide in the two calculations. Since the new model was con-

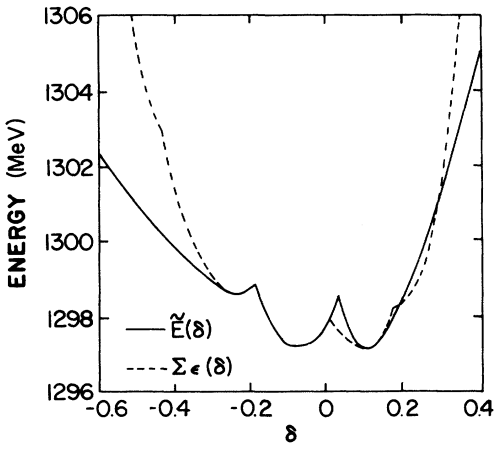

FIG. 2. Comparison of the energy surface obtained from the calculation of $\tilde{E}(\delta)$ and the energy surface obtained from the calculation of $\Sigma\epsilon(\delta)$ for 42 particles. The two energy surfaces are different, but the energies and deformations at the minima are the same for both.

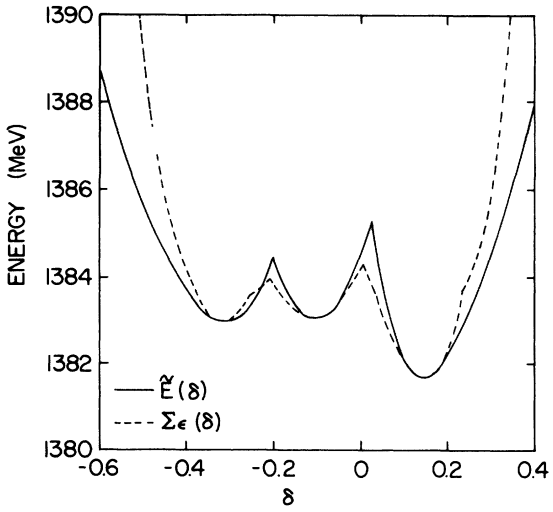

FIG. 3. Comparison of the energy surface obtained from the calculation of $\tilde{E}(\delta)$ and the energy surface obtained from the calculation of $\Sigma\epsilon(\delta)$ for 44 particles. The two energy surfaces are different, but the energies and deformations at the minima are the same for both.

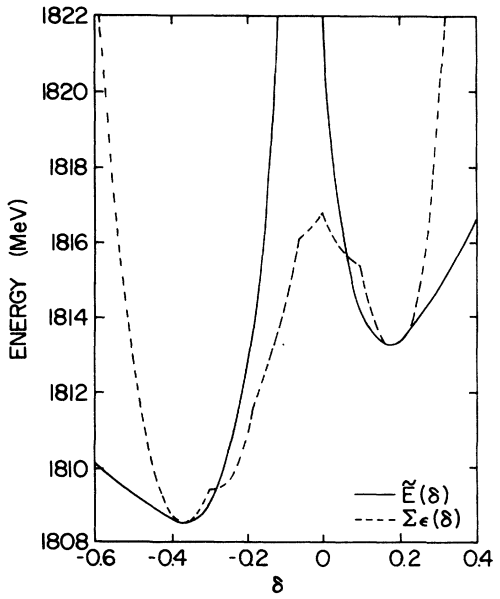

FIG. 4. Comparison of the energy surface obtained from the calculation of $\tilde{E}(\delta)$ and the energy surface obtained from the calculation of $\Sigma\epsilon(\delta)$ for 54 particles. The two energy surfaces are different, but the energies and deformations at the minima are the same for both.

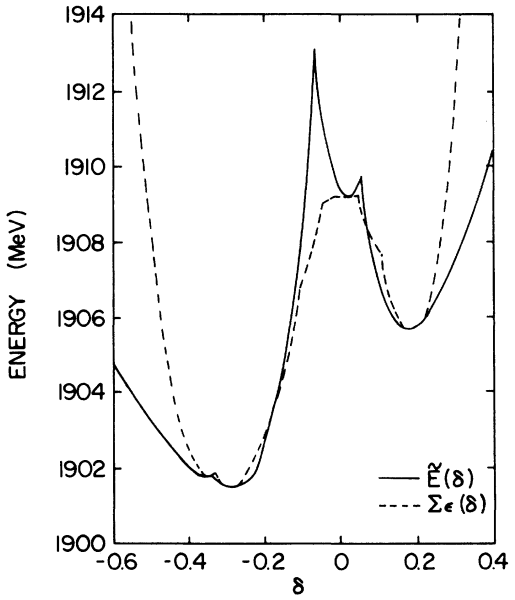

FIG. 5. Comparison of the energy surface obtained from the calculation of $\tilde{E}(\delta)$ and the energy surface obtained from the calculation of $\Sigma\epsilon(\delta)$ for 56 particles. The two energy surfaces are different, but the energies and deformations at the minima are the same for both.

structed specifically to reproduce this feature of the Nilsson model, this is hardly surprising. Second, since the Lagrange multiplier is $(\delta - \delta_{\min})\gamma$, for each configuration, the minima in $\tilde{E}(\delta)$ all occur when Λ is zero, as they must in a valid constrained variational calculation.

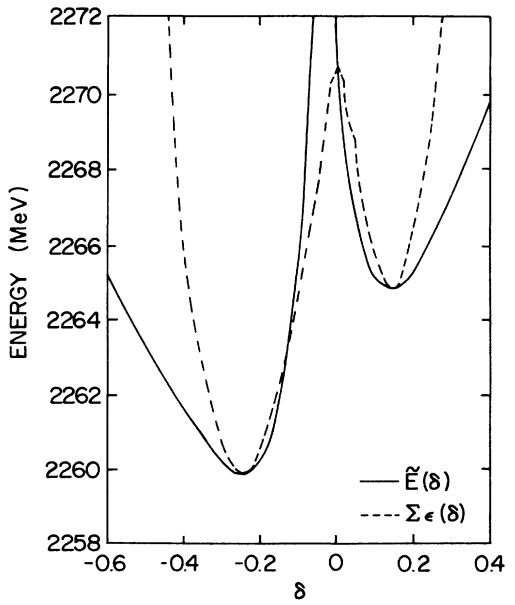

FIG. 6. Comparison of the energy surface obtained from the calculation of $\tilde{E}(\delta)$ and the energy surface obtained from the calculation of $\Sigma\epsilon(\delta)$ for 64 particles. The two energy surfaces are different, but the energies and deformations at the minima are the same for both.

It is also clear from these figures that there is considerable difference between the behavior of the new model energy $[\tilde{E}(\delta)]$ and the Nilsson "prescription-energy" $[\Sigma_\lambda \epsilon_\lambda(\delta)]$ between the minima. Although it is not universally true, in general the crossing of the energy curves for adjacent configurations, shown as cusps in the energy surfaces, are much higher in energy for $\tilde{E}(\delta)$ than for $\Sigma\epsilon(\delta)$. These differences in the effective magnitude of the fluctuations in the energy surface could be extremely significant in certain applications of these models. The fact that these cusps occur at (slightly) different values of δ results from the crossover from one configuration to another being determined differently in the two models. In the Nilsson model, one changes configurations when the highest occupied and lowest unoccupied single-particle energy levels cross. In the modified model these configurations are changed when the configuration which leads to the lowest energy changes. Because of the removal of the Lagrange multiplier in the modified model, these two deformations will not be the same.

One other difference between the two types of curves occurs at the extreme limits of the deformation, for either sign. Because of the form of $\omega(\delta)$ mandated by volume conservation, the Nilsson "energy" goes to infinity at $\delta = -\frac{3}{2}$ or $\delta = +\frac{3}{4}$. Since volume conservation is not imposed in the new model, this sharp rise at the "edges" of the energy surface is not present.

A striking difference between the two models emerges if one plots the energy as a function of the expectation value of Q instead of the artificial quantity δ. This presents no difficulty in the modified model but in the usual Nilsson model the cusps correspond to level crossings and at these points $\langle Q \rangle$ is not continuous. Since there is no prescription to indicate how the energy should be calculated except for summing the lowest $2N$ eigenvalues, there will be gaps in the energy surface corresponding to this discontinuity in $\langle Q \rangle$. This is seen in Fig. 7, where the energy surfaces obtained in the two models are compared as functions of the more natural variable $\langle Q \rangle$. This particular comparison is for 44 particles, but the results are typical. Again, the modified model results are shown with a solid line while the Nilsson results are indicated by the dotted line. As dictated by the construction of the model, the minima coincide. Now, however, the difference between the two models between adjacent minima is even more striking. The Nilsson curve is not defined.

There is another way to remove this difficulty

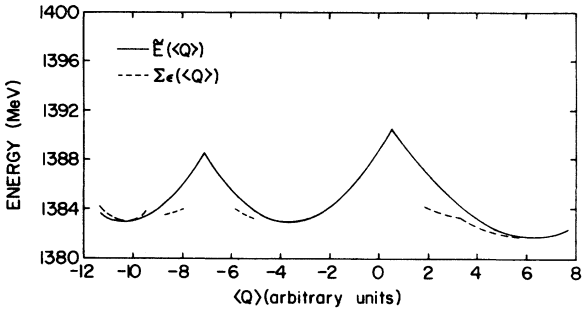

FIG. 7. Comparison of the energy surface obtained from the calculation of $\tilde{E}(\langle Q\rangle)$ and the energy surface obtained from the calculation of $\Sigma\epsilon(\langle Q\rangle)$ for 44 particles. The minima have the same energies and deformations, but much of the energy surface is not defined in the curve of $\Sigma\epsilon(\langle Q\rangle)$.

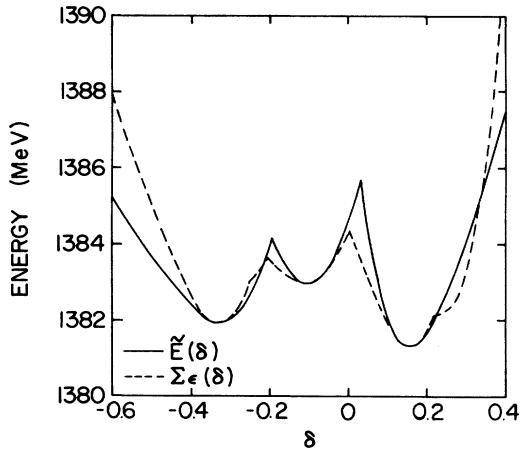

FIG. 8. Comparison of the energy surface obtained from the calculation of $\tilde{E}(\delta)$ and the energy surface obtained from the calculation of $\Sigma\epsilon(\delta)$ for 44 particles with ω_b as a variational parameter. The two energy surfaces are different, but the energies and deformations at the minima are the same for both.

from the usual Nilsson model and that consists of adding a pairing part to the Hamiltonian or, more specifically, to introduce "occupation-probabilities" via a BCS-type formula. The inclusion of pairing smooths out the nonphysical cusps and is essential for certain applications of the Nilsson model. Such an extension of the model is being pursued but because of the additional complexities in a theoretical model containing pairing, this is difficult.

VII. AN ADDITIONAL MODIFICATION

Experience in CHF and other variational calculations, performed in truncated bases, has shown that there is a "hidden" variational parameter which can play an important role. This parameter is the frequency of the oscillator potential used to generate the basis functions. In the Nilsson model there is no distinction made between this and the frequency of the one-body potential in the Hamiltonian. (Thus the dependence of ω on δ, resulting from the imposition of volume conservation, is built into the basis functions.) Because the present calculation is variational in nature, there is an unambiguous way of determining this parameter. The energy should be minimized, for each calculation, with respect to this frequency. The results of such a calculation are shown in Fig. 8. Here both the usual Nilsson model and the modified model have the frequency of the basis ω_b treated as a variational parameter. The minima, in either case, are shifted from the previous positions since those results, with ω_b fixed, are really only valid as the size of the basis goes to infinity.

VIII. CONCLUSION

It has been shown that the Nilsson model can be modified in such a way that the attractive features remain while some of the deficiencies are removed. In particular, the modified model contains an unambiguous procedure for calculating the many-body energy from the single particle Hamiltonian. It has been demonstrated that the results of the two calculations have appreciable differences between the minima and thus may give rather different results in subsequent calculations, such as those of shell effects in deformed nuclei.

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