Effect of unbounded operators on variational calculations in truncated bases

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(Received 21 September 1978)

The validity of the results of finite basis, constrained variational calculations with unbounded operators has remained unquestioned despite the mathematical difficulties in an infinite basis pointed out by Fonte and Schiffrer. It will be shown here that the difficulties associated with unbounded operators are not restricted to infinite bases and that, in fact, the consequences are equally severe in finite bases. The demonstration will be made both for a one dimensional, one body model and in a full three dimensional, many body calculation typical of those currently being employed in nuclear physics. The correct procedure for imposing such constraints, e.g. the quadrupole constraint, and the validity of previous calculations remain open questions.

[NUCLEAR STRUCTURE Nonconvergence of variational calculations studied in finite bases.]

INTRODUCTION

In many areas of physics, variational calculations play a dominant role because direct solutions of the relevant equation, such as the many-body Schrodinger equation, are unobtainable. It is often of interest to impose constraints upon these calculations so that the expectation value of some operator or set of operators will have some prescribed value. Certain operators which are naturally of interest, such as the various multipole operators, have the feature that they are unbounded, either from above, below, or both, i.e., the representation of the operator becomes infinite. Although such operators have been extensively used in variational calculations in truncated, finite bases,[1] Fonte and Schiffrer[2] have shown that the equations solved have *no solution* in an infinite basis. This certainly casts some doubt on the validity of the finite basis results.

Some light was shed on the situation by the theorem proven by Bassichis *et al.*[3] According to this theorem the energy of a wave function with a constrained value of an unbounded operator can be made arbitrarily close to the energy of the ground state. In addition, when a simple, one-body, one-dimensional problem was considered it was shown that the unboundedness of the constrained operator had consequences even in finite basis calculations. It was found, for example, that the compressibility, the resistance of this system to a change in size, was a strong function of the size of the basis employed. In accordance with the theorem, the compressibility decreased by a factor of 2 when the basis was increased from 3 to 5 states and decreased by another factor of 2 with an increase from 5 to 12 states. This dependence was quite consistent with the zero compressibility predicted for an infinite basis.

In spite of these results, constrained variational calculations with unbounded operators continue to be performed in finite bases. Indeed certain results obtained in finite basis, many-body calculations seem to show no evidence whatsoever of this unboundedness difficulty.[4]

Here the simple one-body, one-dimensional model will be considered in detail in order to isolate the source of the difficulties associated with unbounded operators even in finite bases. Thus guided, the many-body calculations will be repeated and shown to exhibit the same features as the simple model. It is hoped that this investigation of the difficulties will lead to a solution to the problem of imposing such constraints in variational calculations.

THE SOURCE OF THE DIFFICULTY

The one-dimensional problem considered earlier[3] (henceforth referred to as I) consisted of a single particle moving in a Gaussian field

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - V_0 e^{-\beta x^2}. \tag{1}$$

One may solve this problem by numerical integration and obtain the quantities of interest here; the ground state energy and the expectation value of x^2 in the ground state ψ. Alternatively one may perform a variational calculation by writing

$$\psi = \sum C_n \phi_n(x), \tag{2}$$

where the ϕ_n are known functions and the coefficients, C_n, are determined by minimizing $\langle H \rangle$.

The difficulty pointed out by Fonte and Schiffrer[2] arises when one imposes on the variational calculation, using the method of Lagrange multipliers,

the constraint that the expectation value of x^2 has some value different from that at the ground state. Then the quantity to be minimized is

$$E_\lambda = \langle\psi|(H-\lambda x^2)|\psi\rangle \tag{3}$$

and since x^2 is unbounded as x goes to infinity, $H-\lambda x^2$ has a continuous spectrum extending to $-\infty$ for positive values of λ. Thus E_λ has no minimum and no solution is possible in an infinite basis. Fonte and Schiffrer thus claim that there is no content to solutions of this minimization problem obtained in finite bases.

In I it was shown that the difficulty was not peculiar to the method of Lagrange multipliers but that the unboundedness of the operator itself implied that the constrained energy, $E_\lambda+\lambda\langle x^2\rangle$, could be made arbitrarily close to the ground state energy, E_0, by constructing wave functions in a particular way. Furthermore it was shown that in this one-dimensional model, the consequences of this theorem were apparent for even small basis calculations. This is shown in Fig. 1. The states used as a basis were the usual harmonic oscillator wave functions

$$\phi_n(x)=\left(\frac{\gamma}{\pi^{1/2}}\frac{1}{2^n n!}\right)^{1/2}H_n(\gamma x)e^{-1/2\gamma^2x^2} \tag{4}$$

and since only even parity states were considered, N is the maximum n divided by 2.

The strength of the potential V_0, its range β, and the other constants can be combined with the oscillator constant γ to yield a single parameter in terms of which everything can be expressed

$$\omega=\hbar\gamma/(2mV_0\beta)^{1/2}.$$

The calculations whose results are shown in Fig. 1

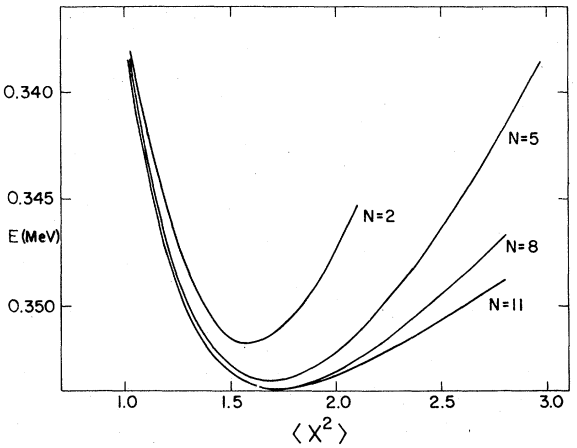

FIG. 1. E vs $\langle x^2\rangle$ with various fixed N. Corresponding to the common practice in many-body calculations, the oscillator parameter ω is held fixed at the value determined in the unconstrained calculation.

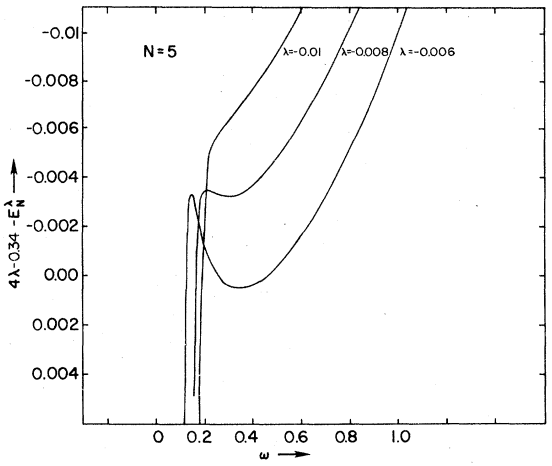

FIG. 2. $(4\lambda-0.34-E_N^\lambda)$ vs ω with $N=5$ and various fixed λ. Here it is seen that there is a local minimum in E_N^λ for some values of λ.

were all carried out with ω held fixed at the value which minimized the energy for $\lambda=0$. (Since V_0 and β simply set the scale, they will henceforth both be set equal to one.)

If, instead, one treats ω as a parameter and carries out the calculations varying ω then, as was also shown in I, there will only be local minima in E_λ for negative values of λ and if λ is taken sufficiently negative, even these local minima disappear. This is shown for $N=5$ in Fig. 2. It is this lack of an absolute minimum in E_λ that renders the problem insoluble according to Fonte and Schiffrer.

In finite basis calculations, however, solutions *will* be obtained for a fixed ω and since the constrained energy $E_\lambda+\lambda\langle x^2\rangle$ is the real quantity of interest the lack of a minimum in E_λ may go unnoticed. This is especially true since one normally determines the optimum value of ω with $\lambda=0$ and then uses this value in the constrained calculations.[5] This, however, is not a valid procedure in a finite basis because ω should be treated as a variational parameter. This becomes more evident if one considers the matrix elements of the unbounded operator x^2 in the harmonic oscillator basis:

$$\langle n|x^2|n'\rangle=\frac{\hbar}{2m\omega}\times\begin{cases}[(n'+1)(n'+2)]^{1/2} & \text{if } n=n'+2,\\ (2n'+1) & \text{if } n=n',\\ [n'(n'-1)]^{1/2} & \text{if } n=n'-2.\end{cases}$$

Clearly all the matrix elements of x^2 go to infinity as $\omega\to 0$. Thus the unboundedness of this operator manifests itself in any finite basis, no matter how small. This was also pointed out by Fonte and Schiffrer.

This is not peculiar to the operator x^2. The one-dimensional analog of any multipole operator, namely x^m for any positive even integer m, will have matrix elements that go to infinity as $\omega \to 0$. This can be seen easily by writing

$$\langle \phi_n(x) | x^m | \phi_n(x) \rangle$$

$$= \frac{\gamma}{\pi^{1/2}} \left(\frac{1}{2^n n!} \right) \int_{-\infty}^{\infty} H_n^2(\gamma x) x^m e^{-\gamma^2 x^2} dx$$

$$= \frac{1}{\gamma^m \pi^{1/2}} \left(\frac{1}{2^n n!} \right) \int_{-\infty}^{\infty} H_n^2(y) y^m e^{-y^2} dy$$

$$= \frac{1}{\omega^{m/2}} \times (\text{a number independent of } \omega).$$

If, on the other hand, one deals with a bounded operator then these matrix elements will not go to infinity. This results from the scale change. Consider, for example, $x^2 e^{-cx^2}$ with c very small.[3] The matrix elements will then be

$$\langle \phi_n(x) | x^2 e^{-cx^2} | \phi_n(x) = \frac{1}{\gamma^2} \frac{1}{\pi^{1/2}} \left(\frac{1}{2^n n!} \right)$$

$$\times \int_{-\infty}^{\infty} H_n^2(y) y^2 e^{-y^2} e^{-cy^2/\gamma^2} dy .$$

The factor now multiplying γ^{-2} goes to zero exponentially as γ goes to zero so that in this limit the matrix elements go to zero. A similar demonstration can be made for any technique for cutting off the operator.

It is therefore apparent that the difficulty with unbounded operators should be evident even in finite basis calculations. There it is crucial to consider all values of the oscillator parameter, or its analog in some other basis, particularly in the neighborhood of that value for which the matrix elements go to infinity. This will now be carried out in detail for the one-dimensional model.

In Fig. 3 is shown the constrained energy $E_\lambda + \lambda \langle x^2 \rangle$ as a function of $\langle x^2 \rangle$ for various values of ω. These were obtained using a range of Lagrange multipliers for each case. Clearly the value of ω which minimizes the energy without constraint is not the optimum value for significantly larger values of $\langle x^2 \rangle$.

This is also shown in Fig. 4 where the constrained energy is shown, as a function of $\langle x^2 \rangle$, for various fixed values of the Lagrange multiplier. The curve with ω fixed at its unconstrained optimum value is included for comparison. For fixed ω there is a maximum value that $\langle x^2 \rangle$ can achieve, corresponding to having the wave function purely in that state ϕ_i for which the matrix element of x^2 is a maximum. Thus obviously, for values of $\langle x^2 \rangle$ exceeding this maximum, different values of ω must be employed. The significance of the results displayed

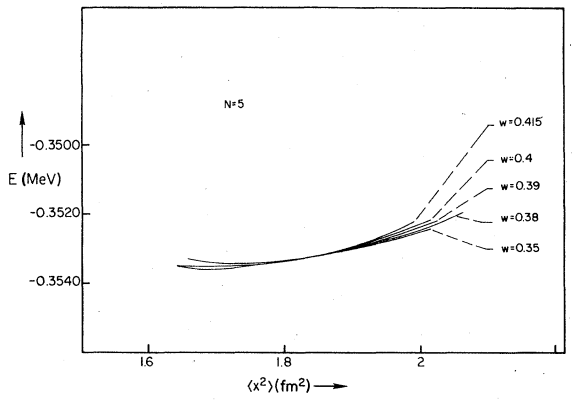

FIG. 3. E vs $\langle x^2 \rangle$ with various fixed ω and $N = 5$. The value of ω which gives the lowest unconstrained energy is 0.415. It is seen that this is not the optimum ω for $\langle x^2 \rangle$ significantly larger than the unconstrained value.

is that energies quite close to the unconstrained ground state energy can be obtained even for these extremely large values of $\langle x^2 \rangle$ by taking sufficiently small Lagrange multipliers. The increasingly large values correspond to decreasingly small values of ω.

For values of $\langle x^2 \rangle$ in the neighborhood of the unconstrained value it is also possible to reach constrained energies well below these obtained with the ω which minimizes the unconstrained energy. In Fig. 5 the constrained energy is shown as a function of $\langle x^2 \rangle$, in the region near the minimum, for various values of the Lagrange multiplier. The curve with fixed ω is again included. The dependence of the energy on the Lagrange multiplier for fixed $\langle x^2 \rangle$ is not monotonic. Energies are, however, attainable which are much closer to the ground state energy than would be obtained with fixed ω. This is shown also in Fig. 6 where the region near the minimum is considered with various fixed values of ω.

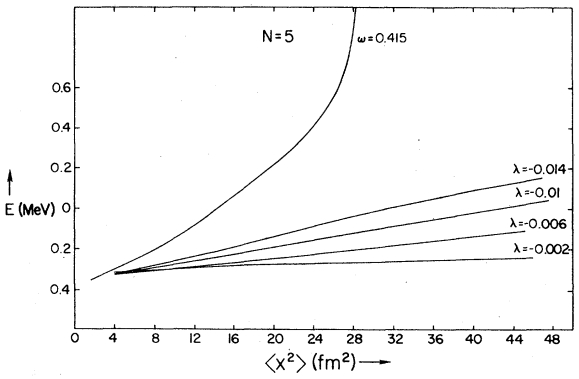

FIG. 4. E vs $\langle x^2 \rangle$ with various fixed λ and $N = 5$. The curve with ω fixed at its optimum value $\omega = 0.415$ is included for comparison.

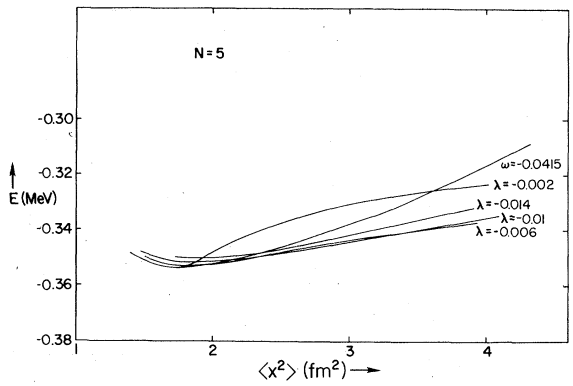

FIG. 5. E vs $\langle x^2 \rangle$ with various fixed λ and $N = 5$ near minimum. The constrained energy is shown as a function of $\langle x^2 \rangle$ in the region near the minimum for various values of the Lagrange multiplier. The curve with fixed ω is again included.

From these results it is clear that the difficulty associated with unbounded operators in an infinite basis is also present in finite basis calculations. One can obtain constrained energies very close to the ground state even for values of the constrained quantity much different than at the minimum. The results of calculations with ω fixed from unconstrained calculations are totally specious. In searching for the lowest energy at a particular value of the expectation value of the constrained operator the oscillator parameter must be varied. If one uses values of the parameter in the vicinity of where the matrix elements of the unbounded operator go to infinity then energies can be obtained which are quite close to the ground state energy.

This effect will now be considered in a full, three-dimensional many-body calculation.

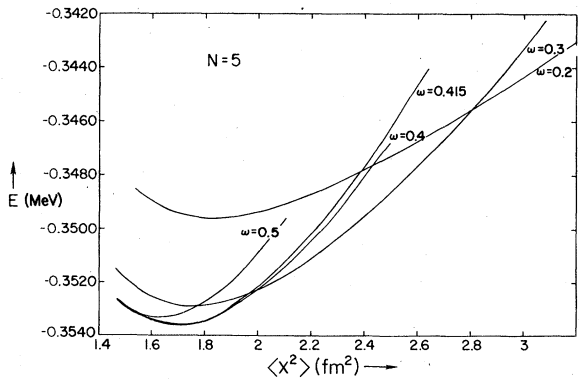

FIG. 6. E vs $\langle x^2 \rangle$ with various fixed values of ω near minimum. The value of ω which minimizes the energy without constraint is not the optimum value even near the minimum.

CONSTRAINED HARTREE-FOCK CALCULATIONS

The Hartree-Fock method has proven useful in many areas of many-body physics. In nuclear physics the method has been used, with constraints added, to calculate moments of inertia,[6] nuclear compressibility,[7] and resistance to quadrupole deformations.[8] In the latter two cases, the operators whose expectation values are constrained are unbounded and thus the variational equations have no solutions if the calculations are carried out in coordinate space, i.e., in an infinite basis. In general, however, such calculations are computationally not feasible and one thus resorts to finite basis calculations. Since the results obtained in the previous section did not explicitly depend on the single-particle or one-dimensional aspects of the problem it would seem apparent that results of such variational calculations with unbounded operators would also be meaningless. However, the equations to be solved are now nonlinear and must be solved by an iteration procedure. It might therefore seem possible for the self-consistent nature of the one-body potential to eliminate the difficulties associated with such operators. It is therefore desirable to examine these calculations in detail.

In early calculations using either a spherical[1] or a deformed[5] harmonic oscillator basis, the effect of the unbounded, constrained operator was not noticed because the optimization of the oscillator parameters was carried out only for the unconstrained solutions. These optimum parameters were then held fixed when the constraint was introduced. The insensitivity of the unconstrained energy to variations in the oscillator constants, in these large basis calculations, gave credence to the incorrect assumption that it was not necessary to optimize the oscillator constant for each value of the Lagrange multiplier. Such assumptions were mandated by the large amount of computer time required for each calculation when complicated, realistic, two-body interactions are employed.

Most recent calculations employ density-dependent, δ function interactions which have the great advantage of computational simplicity.[9] With these forces much larger bases could be used and the interesting question of fission barriers of heavy nuclei could be addressed.[4] Because large deformations must be considered it is natural to use a deformed harmonic oscillator basis, so that there are two parameters to be optimized. The scope of the calculations is so large, however, that the computer time involved becomes quite large even with δ function forces. The optimization was, therefore, not done with sufficient care

and the effects of the unbounded constrained operator were not detected. In fact, as will be shown later, E was certainly not found to be a flat function of the constrained quadrupole moment and, in fact, the function is steeper, in the vicinity of the minimum, in the *larger* basis. These results certainly seem to contradict the theorem proven in I.

The solution to the constrained Hartree-Fock problem involves the diagonalization of the matrix

$$\langle i|h|j\rangle = \langle i|t|j\rangle + \sum_{\mu} \langle i\mu|V_A|j\mu\rangle + \tfrac{1}{2}\sum_{\mu\gamma} \langle \mu\gamma|\phi_i\phi_j\, dV/d\rho|\mu\gamma\rangle - \lambda\langle i|q|j\rangle ,$$

where V_A is taken to be the density-dependent δ function interaction of Skyrme,[10] and λ is the Lagrange multiplier associated with the constrained quadrupole moment. Because q is unbounded, going to $+\infty$ in some directions and $-\infty$ in others, as r goes to infinity, no solution to the equation

$$(h - \lambda q)\phi_\mu = \epsilon_\mu \phi_\mu$$

can be found in an infinite basis. One might expect that this difficulty would not be present in a finite basis because, although

$$\langle \vec{r}|q|\vec{r}\rangle \to \pm\infty \quad \vec{r}\to\infty ,$$

the truncated operator, whose matrix elements enter $\langle i|h|j\rangle$, is

$$\langle r|q|r\rangle_T = \sum_{i,j=1}^{N} \langle r|i\rangle\langle i|q|j\rangle\langle j|r\rangle .$$

Since the harmonic oscillator wave functions, for finite N, fall off exponentially as $|\vec{r}| \to \infty$, this truncated operator would appear to be bounded. This is, however, misleading. The nonzero matrix elements of r^2Y_{20} in a deformed harmonic oscillator basis, nmn_z, are given by

$$\langle nmn_z|q|nmn_z\rangle = \left(\frac{5}{4\pi}\right)^{1/2}\frac{d^{2/3}}{b}\left(\frac{2n_z+1}{2}\right) - \left(\frac{5}{16\pi}\right)^{1/2}\frac{1}{d^{1/3}b^2}(2n+|m|+1),$$

$$\langle n+1mn_z|q|nmn_z\rangle = \frac{1}{d^{1/3}b^2}\left[\frac{5}{16\pi}(n+1)(n+|m|+1)\right]^{1/2},$$

$$\langle nmn_z+2|q|nmn_z\rangle = \frac{d^{2/3}}{b^2}\left[\frac{5}{4\pi}\left(\frac{n_z+1}{2}\right)\left(\frac{n_z+2}{2}\right)\right]^{1/2}.$$

The definitions of d and b are clear from the expression for the wave functions in this basis:

$$\phi_{nmn_z}(r,\phi,z) = Nb^3\eta^{m/2}e^{-\eta/2}L_n^m(\eta) \times e^{-\xi^2/2}H_{n_z}(\xi)e^{im\phi},$$

where

$$N = \left(\frac{n!}{(n+m)!}\right)^{1/2}\left(\frac{1}{\pi^{2/3}2^{n_z}n_z!}\right)^{1/2},$$

$\xi = zb^2/d^{2/3}$, and $\eta = r^2d^{2/3}b^4$.

One sees that there exist regions in the parameter space d and b where the matrix elements $\langle i|q|j\rangle$ themselves go to infinity. Then the matrix elements of the Hartree-Fock Hamiltonian will also be infinite and the expectation value of $H - \lambda Q$ will be unbounded from below.

To examine this numerically, constrained Hartree-Fock calculations were carried out for ^{12}C. The calculations were essentially the same as those used to study heavy nuclei[4] with the following exceptions: First, the advantage of using these simple forces is negated if one includes the Coulomb force properly. One would then have all the usual difficulties in calculating this part of the potential matrix elements for all the oscillator parameters considered and one might just as well use a more complicated nuclear part. Thus the

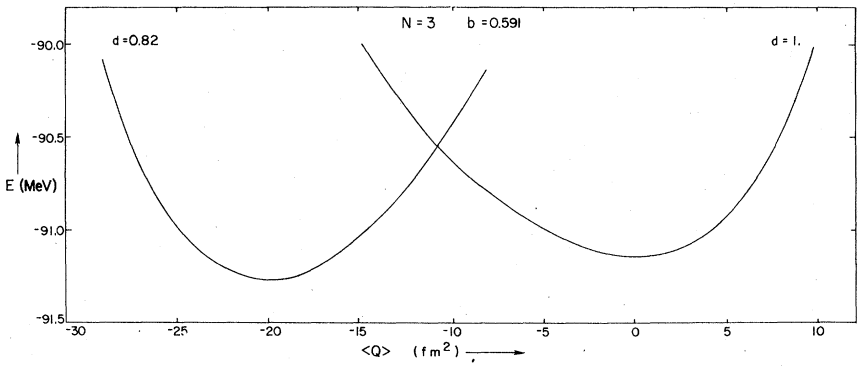

FIG. 7. E vs $\langle Q\rangle$ with $d = 0.82$, $b = 0.591$, $N = 3$, and varying λ. This is an example of the traditional "energy deformation surface" obtained with the parameters as determined at the minimum.

Coulomb force is treated approximately in these types of calculations.[11] Such an approximation will, of course, destroy the relationship between the energy as calculated from

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

and that calculated from the eigenvalues of the Hartree-Fock matrix, ϵ,

$$E = \tfrac{1}{2}\sum_{\lambda} [\langle \lambda | t | \lambda \rangle + \epsilon_\lambda] - \tfrac{1}{2}\sum_{\lambda\mu\gamma} \langle \mu\gamma | \phi_\lambda \phi_\lambda dV/d\rho | \mu\gamma \rangle^{\sim} .$$

Calculation of these two quantities, without any approximation, would supply a useful measure of the degree of convergence of the iteration procedure. Thus in the test calculations reported here, the Coulomb force was entirely neglected.

A second approximation normally made involves pairing effects. Because pairing is known to be important in nuclei one would like to somehow take it into account. A completely self-consistent treatment including pairing, called the Hartree-Bogoliubov method,[12] is not feasible for heavy nuclei. Thus one carries out an approximate calculation, where, for example, a constant pairing gap is assumed, and this again destroys the exact relationship satisfied by the Hartree-Fock quantities. To avoid these approximations, pairing will also be neglected entirely in these test calculations.

The first oscillator basis considered utilized only three harmonic oscillator shells, which at sphericity correspond to the $s_{1/2}$ shell, the $p_{1/2}$-$p_{3/2}$ shell, and the s-d shell. When the basis was made spherical only one minimum was obtained, namely a spherical solution. This is quite different from the results obtained with other interactions where there are prolate and oblate minima for spherical basis calculations[1] but this is just a peculiarity of this interaction. When the basis was deformed a minimum was located with negative quadrupole moment as in earlier calculations with this force.[4] A variation of the oscillator parameters was carried out and optimum values determined for this oblate minimum. One then obtains a "typical" energy deformation surface as is shown in Fig. 7. These are obtained by introducing a Lagrange multiplier λ and solving the variational problem

$$\delta \frac{\langle \psi | (H - \lambda Q) | \psi \rangle}{\langle \psi | \psi \rangle} = \delta E_c = 0$$

for a variety of λ's. With the resulting ψ's one calculates the expectation value of Q and the energy,

$$E = \langle \psi | H | \psi \rangle = E_c + \lambda \langle \psi | Q | \psi \rangle$$

for ψ normalized.

According to the theorem of Bassichis *et al.*, however, one should be able to obtain wave functions whose energy is arbitrarily close to the ground states, with any value of the quadrupole moment. To obtain such states one needs the appropriate Lagrange multiplier and the correct values of the oscillator parameters. Thus in Fig. 8 one sees that by keeping λ fixed and varying b and d one may indeed obtain curves much flatter than the "traditional" curve.

A similar situation exists if one considers larger bases. The results for a space which includes the fourth oscillator shell, the p-f shell, is shown in Fig. 9. Again one finds regions in which the ap-

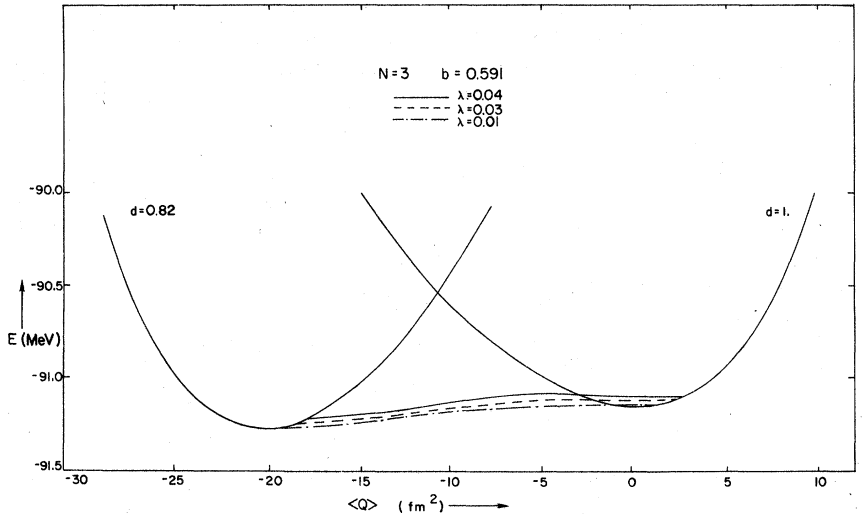

FIG. 8. E vs $\langle Q \rangle$ with $b = 0.591$, $N = 3$, and various fixed values of λ. It is apparent that by varying d for various fixed values of λ one may indeed obtain curves much flatter than the "traditional" curve.

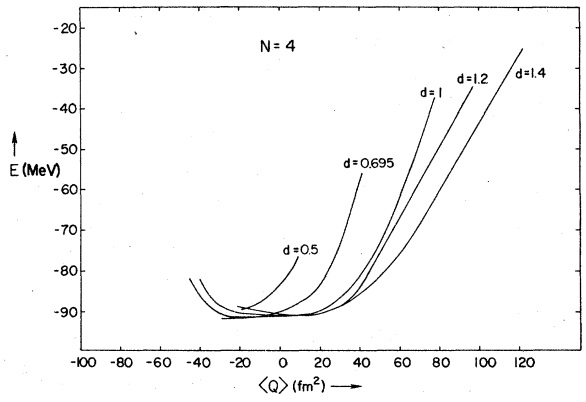

FIG. 9. E vs $\langle Q\rangle$ with various fixed values of d and $N=4$. The curve with d fixed at its optimum value $d = 0.695$ is included for comparison. In each case b was fixed at 0.675 and again one obtains a curve much flatter than the traditional curve.

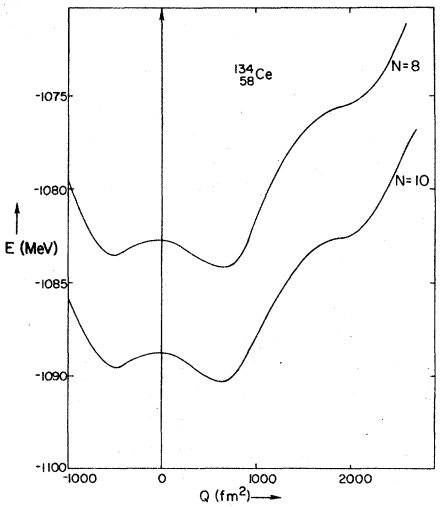

FIG. 10. E vs $\langle Q\rangle$ and $N=8$, 10. These are the results for $^{134}_{58}$Ce obtained by Flocard *et al*. (Ref. 4). There are two striking features of these curves: the curve is definitely not a flat line, and there is no apparent flattening as the space is enlarged, in fact, near the minimum it becomes steeper.

propriate λ, b, and d will yield wave functions with quadrupole moments having diverse values while the energies are quite close to that of the ground state.

The importance of optimizing the oscillator parameters has been stressed in recent work[4] and a systematic approach was taken to insure optimization for each Lagrange multiplier. (A quadratic constraint is employed here but this makes no essential difference.) Six sets of b's and d's were used, in the neighborhood of the unconstrained optimum values, and from the subsequent results the optimum set was obtained. These calculations of a heavy nucleus were carried out using an approximate Coulomb interaction and an approximate treatment of pairing. The resulting energy deformation curve is shown in Fig. 10 for two different bases, $N=8$ and 10. There are two striking features of this curve in the present context. First, the curve has structure, one does not obtain a flat line. Second, there is no apparent flattening as the space is enlarged. Instead the curvature near the minimum seems to be larger for the larger space. This illustrates that the problem of determining the optimum parameters is not as simple as it would appear. It must be born in mind that the equations being solved are nonlinear and questions of stability are nontrivial.

To this point the unboundedness of the operator being constrained has been used to determine the direction in harmonic oscillator space to search in order to find wave functions with energies close to that of the ground state. Because of the apparent discrepancy with the results for the heavier nucleus it was considered worthwhile to seek other effects of the unboundedness. It was found that, in fact, there are consequences in these finite bases which have a drastic effect on any such calculations.

The fact that has been overlooked up until now is that the quantity which must be minimized is

$$E_c = \langle\psi\,|\,(H-\lambda Q)\,|\,\psi\rangle\,.$$

The procedure traditionally followed is to minimize E_c with respect to some variations in the wave functions, namely the expansion coefficients of the single-particle wave functions. Then one minimizes the expectation value of H itself with respect to variations with the oscillator parameters. This is not consistent. One must, according to the variational theorem, minimize the expectation value of some quantity and when constraints are present, that quantity is E_c.

It is when one follows this correct procedure that the Fonte and Schiffrer difficulties appear. One may learn about the behavior of E_c as a function of the oscillator parameters by considering the first matrix element of the Hartree-Fock Hamiltonian. The two critical components are the kinetic energy

$$\langle 1\,|\,t\,|\,1\rangle = d^{1/3}b^2\left(1+\frac{1}{2d}\right)$$

and the λq term

$$\langle 1\,|\,-\lambda q\,|\,1\rangle = -\lambda\frac{1}{3}\frac{1}{b^2 q b d^{1/3}}(d-1)\,.$$

The regions of interest are those where the eigenvalues of the matrix go to negative infinity. From

the λq term it is seen that for λ negative this occurs when d is less than one and either d or b approaches zero. Since the kinetic energy goes to infinity faster than the λq term goes to negative infinity when d goes to zero, the only interesting region is when $b \to 0$.

When λ is positive the region of interest is when d is greater than one and when d goes to infinity or b goes to zero. In either case the λq term dominates the kinetic energy. These cases were chosen for study.

First, d was set equal to 2 and $\lambda = 0.5$. Since the minimum in the energy was found at $b = 0.591$ one might just take a point at a larger b and at a smaller b and if both lead to larger energies assume, quite naturally, that this is the optimum b. In fact there is a local minimum in E_c in this region but the function is not single valued. If one starts with $b = 0.7$ and decreases it in small steps, each time beginning with the previous solution, one obtains the solid curve in Fig. 11 which has a rather flat region and then rises to very large values for small increases in b. If one starts with smaller values of b, such as 0.3 and increases b in small steps, one instead obtains the dotted curve in Fig. 11. The reason for the two branches on the curve is that different single-particle orbitals are being filled. If one begins with the $\frac{1}{2}^+$, $\frac{1}{2}^-$, and $\frac{1}{2}^+$ levels occupied, as will happen with large enough b, these levels will remain the lowest as b is decreased until $b = 0.3$ is reached. If instead,

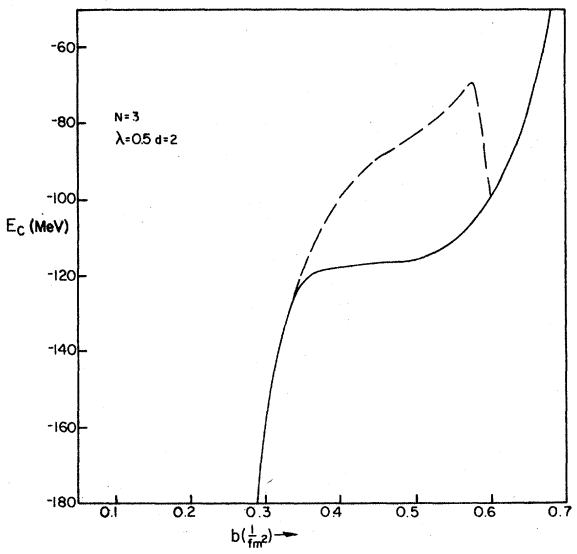

FIG. 11. E_c vs b with $\lambda = 0.5$, $d = 2$, and $N = 3$. The solid curve corresponds to the filling of one set of single-particle orbitals, the dotted curve to another. There is an apparent minimum near the accepted value of b if one starts with the latter configuration and a small b and increases b.

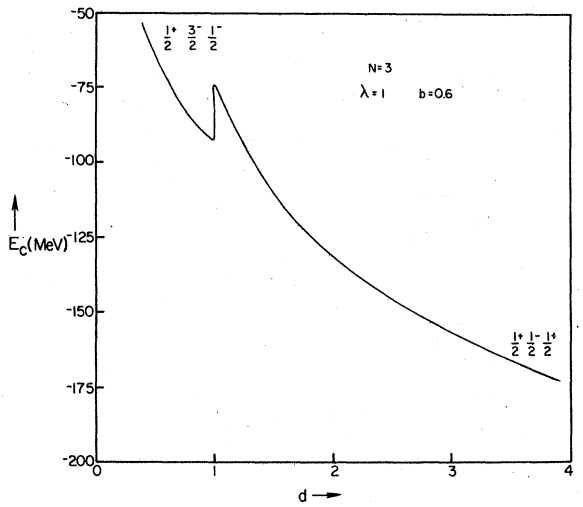

FIG. 12. E_c vs d with $\lambda = 1$, $b = 0.6$, and $N = 3$. The two branches of the function correspond to two configurations of filled single-particle orbitals. Again there is a local minimum but no real solution.

one begins with $b = 0.3$, the $\frac{1}{2}^+$, $\frac{1}{2}^-$, and $\frac{3}{2}^+$ levels will be occupied and they will remain the lowest as b is increased until $b = 0.6$. Because of this complicated structure the curve seems to display a E_c minimum near $b = 0.6$. What is significant, however, is that no matter how one starts, E_c goes to $-\infty$ as b goes to zero and if one performs a thorough search for the minimum in E_c, instead of just checking a few points, one can only conclude that the equations have no solution. Larger and larger negative E_c will be obtained for smaller

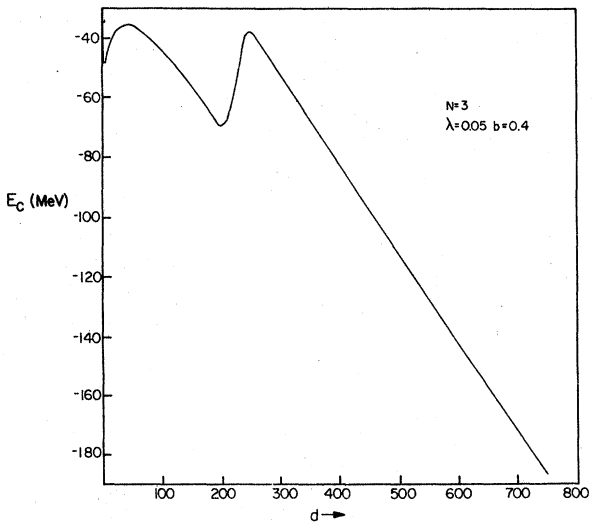

FIG. 13. E_c vs d with $\lambda = 0.05$, $b = 0.4$, and $N = 3$. For this very small Lagrange multiplier one must go to very large values to d before E_c tends to negative infinity. On the way a number of local minima are encountered.

and smaller b's until the limits of the computer are exceeded.

A similar phenomenon exists when one studies E_c as a function of d. With a relatively large value of λ, $\lambda = 1$, and $b = 0.6$ there is again a local minimum for a value of d near that which minimizes the energy. Again it corresponds to the crossover in two branches of a function, as is shown in Fig. 12. There it is again seen that any search for a minimum in E_c would yield no solution.

Finally, in Fig. 13 the results are shown when a typical Lagrange multiplier is used instead of the large one just employed. Here one has to go to huge values of d before E_c tends towards negative infinity. There is quite a bit of structure, maxima and minima, in the region between $d = 1$ and 2, which does not show on this graph. What can be seen is sufficient to demonstrate the difficulty. Even if one correctly minimized E_c instead of E one might incorrectly conclude that there were a solution to the problem. One has to know what region to look in, in order to see that the Fonte and Schiffrer difficulty indeed exists.

CONCLUSIONS

It has been demonstrated that the unbounded nature of a constrained operator will have profound effects on the results of variational calculations even in finite bases. If one carries out the minimization in the traditional manner, optimizing the expansion coefficients by E_c but the oscillator parameters according to E, the effect demonstrated is a flattening of the energy deformation curve. Although one cannot obtain the totally flat curve predicted for an infinite basis, one can get points well below the usual curve. More severe is the result of a consistent minimization of the constrained Hamiltonian's expectation value. Then it has been demonstrated that for any Lagrange multiplier there is no solution to the optimization problem. Instead there is some direction in the space of oscillator parameters for which E_c goes to negative infinity.

The source of the difficulty in finite basis calculations is that the matrix elements of an unbounded operator are themselves unbounded. The obvious solution to this mathematical dilemma is to insert a factor which artificially puts a bound on the operator in coordinate space, such as $e^{-\beta r^2}$. This would put a bound on the matrix elements and would then have a minimum. The results would be meaningless, however, unless they were independent of β. This was not so for the one-dimensional case. Instead the solution must be in constraining some other operator besides the quadrupole, or other multipoles. One possibility is to employ just the angular part of the various multipole operators. This is, in fact, more complicated, computationally, than using the full operator and, in effect, corresponds to a particular form of cutoff for which there is no physical significance. The correct procedure seems, therefore, to be still an open question.

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