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# Bounded quadrupole operator for constrained variational calculations

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A bounded operator is introduced so that rigorous constrained variational calculations can be performed. With this operator the calculations are no more complex than previous, nonrigorous calculations and no dependence on unphysical parameters is introduced. It is shown that results previously obtained in a mathematically invalid way are, to a large extent, reproduced by these valid calculations.

[NUCLEAR STRUCTURE Modified constraint introduced for calculation of nuclear deformation energy.]

## INTRODUCTION

Some time ago Fonte and Schiffrer[1] pointed out that the accepted practice of using the quadrupole operator in constrained variational calculations was not a valid mathematical procedure. This was based on the observation that $Q=r^2Y_{20}$ was unbounded both from above and below and would therefore lead to infinitely attractive external potentials, at infinity, in calculations with Lagrange multipliers. It was later shown that this difficulty manifested itself even in constrained Hartree-Fock calculations in truncated spaces, where the unboundedness of $Q$ was less apparent.[2] This cast doubt on the reliability of predictions based on the results of such calculations of nuclear "energy-deformation surfaces.[3]"

A solution to this problem was put forth in the original work of Fonte and Schiffrer, where it was suggested that a cutoff be introduced so that the external potential does not extend beyond the nuclear surface. Inserting such a cutoff in actual calculations was shown,[4] however, to introduce a dependence on the cutoff length which was unacceptable given the ambiguity in its definition. An alternate solution was also suggested by Fonte and Schiffrer in which the mass distribution was specified by certain inequalities. It would be preferable if the difficulty were overcome in a way that was simple to implement. Furthermore, one would like to investigate to what extent those results already obtained, by performing calculations that were not rigorously correct, were valid. In these respects, the solution put forth by Giraud and Le Tourneux[5] is also not satisfactory. They suggest the addition of a second constraint—on the square of the quadrupole operator. Although this procedure can eliminate the problem caused by an external potential which goes to minus infinity, one would then be faced with the calculation of a two-body operator's matrix elements instead of a one body operator. This would constitute a serious handicap, and it is therefore not surprising that calculations using this procedure have not been carried out.

Here it will be shown that one may introduce a modified constraint which has all of the desired features; it is simple to implement, introduces no new parameters, and is useful in determining the validity of the results of previous, nonrigorous calculations.

## THE MODIFIED CONSTRAINT

The usual constrained variational calculation involves the minimization of the Hamiltonian

$$H_Q=H-\lambda_Q Q\ ,$$

where $H$ is the Hamiltonian, $\lambda_Q$ the Lagrange multiplier, and $Q$ is the quadrupole operator, $r^2Y_{20}$. The lack of a solution follows from the property that letting the system extend to infinity, in some direction, will lead to infinitely large, negative values of the expectation value of $H_Q$, $\mathscr{E}$.

Since one wishes to limit the extent of the system whose deformation is being considered, one rather

obvious possibility is the introduction of a second constraint on, for example, the expectation value of $r^2$. Because this is a one-body operator, closely related to the quadrupole operator, it will not introduce the complexity that would accompany a quadratic constraint[5] nor will it, as will be shown, introduce any undetermined constant, such as a cutoff length. Since $r^2$ is itself an unbounded operator, one would encounter the same difficulty as with $Q$ if one considered the constrained Hamiltonian

$$H_R = H + \lambda_R r^2 .$$

Here no minimum would exist for $\lambda_R < 0$, since $r^2$ is unbounded from above. However, the constraint is not being imposed on $H$. Rather, to the problem of minimizing the expectation value of

$$H_Q = H - \lambda_Q Q$$

from some *fixed* value of $\lambda_Q$, one imposes the constraint that $\langle r^2 \rangle$ be less than some finite, but *unspecified* value. Since $\langle r^2 \rangle$ will obviously be infinite for a wave function with infinite extent, this implies that the total external potential be bounded. Thus the Hamiltonian to be minimized, for a fixed $\lambda_Q$, is

$$\mathscr{H} = H - \lambda_Q Q + \lambda_R r^2$$

and only values of $\lambda_R$ can be considered which result in

$$-\lambda_Q Q + \lambda_R r^2$$

being bounded from below. Specifically, since the quadrupole operator is

$$Q = 2z^2 - \rho^2 \quad (\text{suppressing } \sqrt{5/16\pi}) ,$$

and since

$$r^2 = z^2 + \rho^2 ,$$

the values of $\lambda_R$ of interest satisfy

$$\lambda_R \geq 2\lambda_Q \quad \text{for } \lambda_Q > 0$$

and

$$\lambda_R \geq -\lambda_Q \quad \text{for } \lambda_Q < 0 .$$

The expectation value of $\mathscr{H}$, designated by $\mathscr{E}_R$, will be a function of $\lambda_R$. In the usual application of Lagrange multipliers, the value of $\lambda_R$ would be determined by requiring $\langle r^2 \rangle$ to have some prescribed value. Here, instead, $\lambda_R$ is to be determined by the requirement that $\mathscr{E}_R$ be minimized. This is possible because the purpose of the $r^2$ constraint is to exclude solutions with infinite extent and this is accomplished for any $\lambda_R$ satisfying the inequalities. Thus, since $r^2$ is a positive definite operator and since only positive values of $\lambda_R$ satisfy the inequalities, the minimum allowable value of $\lambda_R$ is the optimal choice.

The constrained Hamiltonian thus becomes

$$\mathscr{H} = H - \lambda_Q Q + 2\lambda_Q r^2 \quad \text{for } \lambda_Q \geq 0$$

and

$$\mathscr{H} = H - \lambda_Q Q - \lambda_Q r^2 \quad \text{for } \lambda_Q \leq 0 .$$

Because the external potential thus defined is bounded from below its matrix elements will also be bounded from below. In the deformed harmonic oscillator basis, for example,

$$\langle nmn_z \mid -\lambda_Q Q + \lambda_R r^2 \mid nmn_z \rangle$$

$$= b^{-2} d^{2/3} (2n_z + 1) \left[ -\lambda_Q + \frac{\lambda_R}{2} \right]$$

$$+ b^{-2} d^{-1/3} (2n + |m| + 1)(\lambda_Q + \lambda_R) ,$$

where $b$ is the volume parameter and $d$ the deformation parameter.[3] For any value of $\lambda_R$ satisfying the inequality, the quantities $(-\lambda_Q + \lambda_{R/2})$ and $(\lambda_Q + \lambda_R)$ are positive so that the matrix elements are bounded from below for all values of $b$ and $d$. Thus solutions to the constrained variational problem in an oscillator basis will exist for any $b$ and $d$, and these parameters may properly be determined by the condition that the constrained energy be minimized.

## NUMERICAL ILLUSTRATION

The procedure suggested here will be demonstrated for the many body, Hartree-Fock calculation studied in detail with a single constraint.[2] Constrained Hartree-Fock calculations were carried out for $^{12}C$ using the Skyrme interaction[6] in the deformed harmonic oscillator basis with three shells. For simplicity, Coulomb effects and pairing were ignored. Previously, without introducing the second constraint, i.e., with $\lambda_R = 0$, the expectation value of the constrained Hamiltonian had no absolute minimum as a function of the oscillator parameter $d$. This is shown in Fig. 1. An "optimum" value of $d$ could erroneously be obtained by calculating the energy,

$$\langle H \rangle = \mathscr{E} + \lambda_Q \langle Q \rangle ,$$

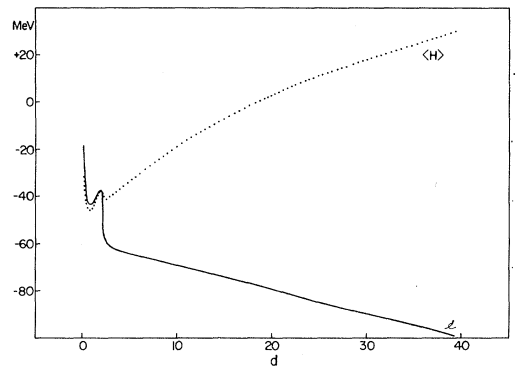


FIG. 1. The constrained energy and $\langle H \rangle$ as a function of $d$. The quantity which should be minimized is $\mathscr{E}$, and although it has a local minimum, no absolute minimum exists. The quantity normally minimized is $\langle H \rangle$ but this does not correspond to correctly solving the variational equations.

and finding the minimum of this quantity. This is not a valid procedure, since in the method of Lagrange multipliers it is $\mathscr{E}$ itself which must be minimized. Nevertheless, $\langle H \rangle$ does have an absolute minimum, as is shown in Fig. 1, and this procedure, through not mathematically valid, was followed in many calculations of nuclear properties.[3]

If one introduces the constraint on $r^2$ into these calculations, then the expectation value of $\mathscr{H}$ does exhibit an absolute minimum. This is shown in Fig. 2. In arbitrary units the quadrupole Lagrange multiplier $\lambda_Q$ was fixed at 0.05. Thus, since $\lambda_R$ must be twice $\lambda_Q$ according to the suggested procedure, the solid line, calculated with $\lambda_R = 0.1$, is the quantity of interest. Here $\langle \mathscr{H} \rangle$ happens to have a second minimum at a value of $d$ much larger than the optimal one, but the $d$ at the absolute minimum is quite close to the result of the invalid calculation. The dependence of $\langle \mathscr{H} \rangle$ on $\lambda_R$ is also shown in Fig. 2. If $\lambda_R < 0.1$ the minimum is only relative with $\langle \mathscr{H} \rangle$ going to negative infinite for infinitely large $d$.

Although the various quantities shown in Fig. 2 are grossly different for most values of $d$, for small values of $d$ their dependence on $d$ is quite similar. This is shown in Fig. 3. The curve labeled $\mathscr{E}_R$ is the expectation value of the constrained Hamiltonian with $\lambda_R = 0.1$. The curve labeled $\mathscr{E}$ is the same quantity with no radial constraint, i.e., $\lambda_R = 0$. The curve labeled $E$ is the energy obtained from $\mathscr{E}$ by adding back the constraint energy, $\lambda_Q Q$. It is the latter quantity which was previously minimized to obtain the optimal value of $d$. Of course one should minimize $\mathscr{E}$ if one is considering bounded operators or, in this case, $\mathscr{E}_R$. As can be seen from the figure, the dependence of these quantities of $d$ is quite similar and the resulting optimal $d$ would be nearly the same for any minimization. In spite of this the minimization of $E$ and $\mathscr{E}$ are, in principle, not correct procedures. For the former, one is not solving the variational equations, while for the latter no absolute minimum exists.

In Table I the properties of the wave functions corresponding to the usual procedure and the sug-

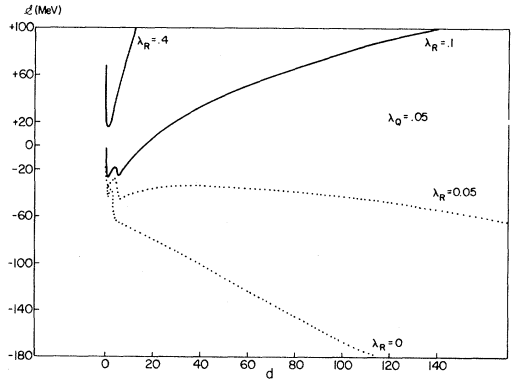


FIG. 2. Results with the modified constraint. The quantity which should be minimized is the expectation value of the constrained Hamiltonian. This quantity is shown, for various values of $\lambda_R$, as a function of $d$. The curve labeled $\lambda_R = 0.1$ is the only meaningful result. The others are included for illustrative purposes.

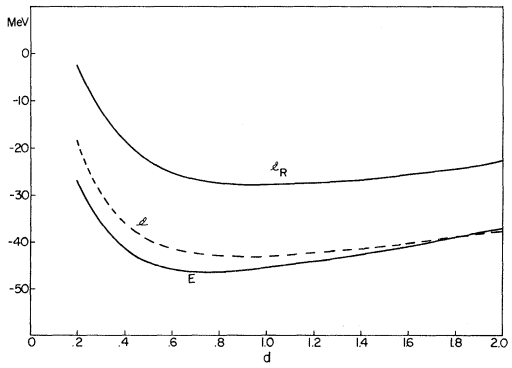


FIG. 3. Comparison of different results. Here it is seen that $\mathscr{E}_R$, a rigorous solution to the variational equations, and $\mathscr{E}$, a quantity which goes to negative infinity for large $d$, have similar dependence on $d$ for small values of $d$. The quantity $E$ is the quantity normally minimized in a constrained calculation.

TABLE I. Comparison of calculated quantities. The energy, quadrupole moment, and radius obtained with the modified constraint, labeled "new," are compared to the corresponding quantities obtained by the usual calculations. Note that only for very large $d$ is there any appreciable difference in these quantities. The latter wave function is not, however, a solution for the variational equations.

| | (MeV) | | (fm$^2$) | | (fm) | |
|---|---|---|---|---|---|---|
| $d$ | $E_{\text{old}}$ | $E_{\text{new}}$ | $Q_{\text{old}}$ | $Q_{\text{new}}$ | $R_{\text{old}}$ | $R_{\text{new}}$ |
| 0.2 | −26.73 | −26.71 | −170.49 | −170.28 | 4.18 | 4.17 |
| 0.4 | −41.87 | −41.84 | −119.12 | −118.82 | 3.82 | 3.81 |
| 0.6 | −45.70 | −45.66 | −89.99 | −89.61 | 3.66 | 3.66 |
| 0.8 | −46.29 | −46.26 | −68.67 | −68.25 | 3.57 | 3.57 |
| 1.0 | −45.59 | −45.55 | −51.32 | −50.92 | 3.52 | 3.52 |
| 1.2 | −44.04 | −44.24 | −35.91 | −36.04 | 3.50 | 3.50 |
| 1.4 | −42.64 | −42.62 | −22.98 | −22.82 | 3.48 | 3.48 |
| 1.6 | −40.86 | −40.85 | −10.67 | −10.77 | 3.48 | 3.48 |
| 1.8 | −39.01 | −39.01 | + 0.91 | + 0.37 | 3.48 | 3.48 |
| 2.0 | −37.11 | −37.15 | + 12.14 | + 10.85 | 3.49 | 3.49 |
| 10.0 | −18.68 | −18.65 | + 1010.42 | + 1010.61 | 6.80 | 6.80 |
| 20.0 | + 2.34 | + 2.34 | + 1628.48 | + 1627.00 | 8.46 | 8.45 |
| 50.0 | + 39.54 | + 39.43 | + 3034.08 | + 3028.00 | 11.37 | 11.36 |
| 100.0 | + 76.44 | + 76.14 | + 4840.59 | + 4824.54 | 14.28 | 14.26 |
| 200.0 | + 123.09 | + 122.34 | + 7710.0 | + 7670.7 | 17.98 | 17.93 |
| 500.0 | + 337.46 | + 202.22 | + 17985.0 | + 14138.0 | 27.40 | 24.30 |

gested modified constraint are compared. The former, which are in principle not valid are labeled "old" while the latter are labeled "new." Small differences in quantities other than the quantity being minimized are not significant since they are not determined variationally and thus may be less stable. The "energy" should converge more quickly than other quantities and, since the iteration procedure is halted when a certain degree of self-consistency is obtained in it, there is some uncertainty in these other quantities. It is significant to note that, except for extremely large values of $d$, there is no essential difference between the quantities calculated with the old and new wave functions. It is, of course, this region of the parameter space, with unreasonably large values of $R$, one wishes to exclude.

## CONCLUSION

It has been shown here that it is possible to introduce a further constraint in deformed variational calculations so that rigorous solutions to the resulting equations do exist. The additional constraint introduces no complexity to the calculations because the operator involved is a one-body operator which is closely connected to the quadrupole moment operator. Furthermore, no new parameters are introduced, such as a cutoff distance, because the Lagrange multiplier associated with the additional constraint is determined uniquely by an optimization condition.

Finally, it has been shown that the traditional method for obtaining solutions, even when no rigorous solution exists, yields results quite close to those obtained by a mathematically correct procedure. This can be understood by the following considerations. The constrained Hartree-Fock Hamiltonian, $h_Q$, is given

$$h_Q = h_0 - \lambda_Q q = h_0 - \lambda_Q (2z^2 - \rho^2)$$
$$= h_0 - 2\lambda_Q r^2 + 3\lambda_Q \rho^2 ,$$

where $h_0$ is the usual unconstrained Hartree-Fock Hamiltonian. For $\lambda_Q > 0$, the modified constraint leads to the Hamiltonian

$$h_{\text{new}} = h_0 - \lambda_Q q + \lambda_R r^2$$
$$= h_0 - \lambda_Q q + 2\lambda_Q r^2$$
$$= h_0 + 3\lambda_Q \rho^2 .$$

Thus the nonspherical part of the external potential is the same in the two calculations. From perturbation expansion arguments it then follows that the admixture into the unconstrained wave functions of basis states with different angular properties will be the same and thus the wave functions should indeed be similar. The effect of the different spherical parts in the external potentials should be small since the spherical part of $h_0$ would normally be very large.

The same argument holds for negative values of $\lambda_Q$. Then

$$h_Q = h_0 + 3\lambda_Q r^2 - 3\lambda_Q z^2$$

and, since $\lambda_R = -\lambda_Q$,

$$h_{\text{new}} = h_0 - \lambda_Q(2z^2 - \rho^2) - \lambda_Q(z^2 + \rho^2)$$
$$= h_0 - 3\lambda_Q z^2 .$$

In spite of this rather fortuitous result, it is clearly preferable to introduce the additional constraint and minimize the correct quantity.

Finally, it should be noted that the introduction of the volume conservation in the Nilsson model is a way of solving the related divergence of the energy in that model. There the coefficients of the spherical and deformed parts of the one-body potential, analogous to $\lambda_R$ and $\lambda_Q$, are not related until volume conservation is imposed. Without such a relation a similar phenomena occurs; there is no minimum in the quantity being minimized.[7]

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