Center-of-Mass Motion and Angular Momentum Projection*

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(Received 22 February 1973)

The results of calculations of rotational energies contain unphysical contributions from the rotation of the center-of-mass part of the wave function. A simple method is presented to remove those unphysical contributions in the case of projected Hartree-Fock calculations. Corrections to several existing Hartree-Fock calculations are computed.

For a finite many-body system the Hamiltonian separates into the sum of two operators, one dependent on center-of-mass variables only, and one which depends only on the intrinsic coordinates,

$$H = H^{\text{c.m.}} + H^{(\text{int})} . \tag{1}$$

This implies that the physical wave function has the form of a product of two factors, one dependent upon the center-of-mass coordinate $\vec{R}$ alone, and the other dependent on the intrinsic coordinates $\vec{\xi}_i$. Thus we may write the wave function as

$$\Psi(\vec{R}, \vec{\xi}_i) = F(\vec{R})\Psi^{(\text{int})}(\vec{\xi}_i) . \tag{2}$$

On physical grounds, we know that the energies associated with a rotational band must arise from a rotation of the intrinsic wave function, $\Psi^{(\text{int})}(\vec{\xi}_i)$, alone. However, in calculations of rotational energies, the wave functions used do not factor as in Eq. (2), and the full wave function $\Psi(\vec{R}, \xi_i)$ is used in place of the wave function $\Psi^{(\text{int})}(\vec{\xi}_i)$. This use of an unfactorable $\Psi(\vec{R}, \vec{\xi}_i)$ leads to unphysical contributions to the energies arising from the rotation of the center-of-mass parts of the wave functions.

We examine this problem for the case in which one uses the method of projecting states of good total angular momentum[1] from an axially symmetric, Hartree-Fock wave function. We show that under certain simplifying assumptions, the unphysical contributions of the center-of-mass parts of the wave function can be removed by simple matrix inversion.

The method of angular momentum projection consists of using the relationship

$$|\Psi^J_{MK}\rangle = \frac{1}{N_{JK}^{1/2}} \frac{2J+1}{8\pi^2} \int d\Omega\, D^{J*}_{MK}(\Omega) R(\Omega) |\phi_K\rangle , \tag{3}$$

to project a state of good total angular momentum, $|\Psi^J_{MK}\rangle$, from a state, $|\phi_K\rangle$ which is not an eigenstate of the total angular momentum. The wave function is normalized, since

$$N_{JK} \equiv \frac{2J+1}{8\pi^2} \int d\Omega\, D^{J*}_{KK}(\Omega) \langle \phi_K | R(\Omega) | \phi_K \rangle . \tag{4}$$

Here $D^J_{MK}(\Omega)$ is the Wigner D function given by

$$D^J_{MK}(\Omega) = \langle JM | R(\Omega) | JK \rangle , \tag{5}$$

where $R(\Omega)$ is the rotation operator, which in turn may be expressed in terms of the three Euler angles α, β, and γ as

$$R(\Omega) = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z} . \tag{6}$$

The energy is then calculated by taking the expectation value of the Hamiltonian, H, with the states $|\Psi^J_{MK}\rangle$, i.e.,

$$E^J_K = \langle \Psi^J_{MK} | H | \Psi^J_{MK} \rangle . \tag{7}$$

Calculations of the energies E^J_K have been carried out for several light nuclei with $|\phi_K\rangle$ generated from Hartree-Fock calculations.[2-4] In these calculations center-of-mass contributions to the energies may enter through two types of errors. First, the full Hamiltonian H may have been used in place of the intrinsic Hamiltonian $H^{(\text{int})}$, where $H^{(\text{int})}$ is

$$H^{(\text{int})} = H - \frac{P^2}{2Am} \tag{8}$$

and $\vec{P}$ is the total momentum operator. Second, the projection in Eq. (3) may be taken to be a projection onto *total* angular momentum. The physical energies are, however, the energies of the intrinsic states, which are eigenfunctions of the *intrinsic* angular momentum. We shall first see how to correct for the error arising from the use of H in place of $H^{(\text{int})}$.

The expectation value of $H^{(\text{int})}$, taken with the states $|\Psi^J_{MK}\rangle$, is

$$\langle \Psi^J_{MK} | H^{(\text{int})} | \Psi^J_{MK} \rangle = \langle \Psi^J_{MK} | H | \Psi^J_{MK} \rangle - \langle \Psi^J_{MK} | \frac{P^2}{2Am} | \Psi^J_{MK} \rangle . \tag{9}$$

We now employ the definition of $|\Psi^J_{MK}\rangle$, Eq. (1), and the orthonormality and addition theorem for the D functions given by

$$\int d\Omega\, D^J_{M'K'}(\Omega) D^{J*}_{MK}(\Omega) = \frac{8\pi^2}{2J+1}\,\delta_{MM'}\,\delta_{K'K}\,, \tag{10}$$

and

$$D^J_{M'K}(\Omega_1) = \sum_\mu D^J_{M'\mu}(\Omega_2) D^J_{K\mu}(\Omega_3)\,, \tag{11}$$

where the angles Ω_1, Ω_2, and Ω_3 are related by

$$R^{-1}(\Omega_1)R(\Omega_2) = R(\Omega_3)\,. \tag{12}$$

These immediately give the result that the center-of-mass term in Eq. (9) is

$$\langle \Psi^J_{MK}| \frac{P^2}{2Am} |\Psi^J_{MK}\rangle = \frac{(2J+1)}{8\pi^2 N_{JK}} \int d\Omega\, D^{J*}_{KK}(\Omega) \times \langle \phi_K | \frac{P^2}{2Am} R(\Omega) | \phi_K \rangle\,. \tag{13}$$

At this point we must make some simplifying assumptions concerning the wave function $|\phi_K\rangle$. First, we assume that $|\phi_K\rangle$ factors into an intrinsic term multiplied by a term which is dependent only on the center-of-mass coordinate, so that

$$\langle \vec{R}, \vec{\xi}_i | \phi_K \rangle = F(\vec{R})\phi^{(\mathrm{int})}(\vec{\xi}_i)\,. \tag{14}$$

This is known to be nearly correct for spherical Hartree-Fock wave functions. In the spherical case, $F(\vec{R})$ is well approximated by the ground-state wave function of the harmonic-oscillator basis being used.[5] Thus, for the nonspherical case, it is reasonable to assume that $F(\vec{R})$ is approximately the ground-state function of a distorted harmonic oscillator. We assume that the distortion is volume conserving and that the center-of-mass density has the same general shape as the total density. This enables us to equate the quadrupole deformation (defined by the ratio of the mean value of the quadrupole moment to the mean value of the monopole moment) of the center-of-mass wave function to the total quadrupole deformation. This completely specifies $F(\vec{R})$ as

$$F(\vec{R}) = N^{-1/2} e^{-a^2X^2} e^{-a^2Y^2} e^{-b^2Z^2}\,, \tag{15}$$

where

$$N = \frac{\pi^{3/2}}{a^2 b}\,, \tag{16}$$

$$b = \left(\frac{1-\frac{1}{2}\mathfrak{D}}{1+\mathfrak{D}}\right)^{1/3} \left(\frac{m\omega}{\hbar}\right)^{1/2}, \tag{17}$$

$$a^2 = \left(\frac{m\omega}{\hbar}\right)^{3/2} / b\,, \tag{18}$$

and where $\mathfrak{D}$ is the quadrupole deformation given by

$$\mathfrak{D} = \frac{\langle \phi_K | (2Z^2 - X^2 - Y^2) | \phi_K \rangle}{\langle \phi_K | (X^2+Y^2+Z^2) | \phi_K \rangle}\,. \tag{19}$$

We may expand $F(\vec{R})$ in states of good angular momentum, as

$$F(\vec{R}) = \sum_L F_L(R) Y_{L0}(\hat{R})\,. \tag{20}$$

If we notice that the rotation operator $R(\Omega)$ is expressible as a product of the center-of-mass rotation operator, $R^{\mathrm{c.m.}}(\Omega)$, and the intrinsic rotation operator, $R^{(\mathrm{int})}(\Omega)$, we have

$$\langle \Psi^J_{M0}| \frac{P^2}{2mA} |\Psi^J_{M0}\rangle = \frac{(2J+1)}{8\pi^2 N_{J0}} \int d\Omega \int d^3\vec{R} \int d^{3A-3}\vec{\xi} \sum_L \sum_{L'} D^{J*}_{00}(\Omega) F_{L'}(R) Y^*_{L'0}(\hat{R}) \frac{P^2}{2Am} \times R^{\mathrm{c.m.}}(\Omega) F_L(R) Y_{L0}(\hat{R}) \phi^{*(\mathrm{int})}(\vec{\xi}) R^{(\mathrm{int})}(\Omega) \phi^{(\mathrm{int})}(\vec{\xi})\,, \tag{21}$$

where we have considered the case $K=0$ for simplicity.

TABLE I. The Hartree-Fock energies and their corrected values for ^{20}Ne as computed from the Hartree-Fock calculation of Ref. 3 for $\alpha = 0.518$ fm^{-1} and $\mathfrak{D} = 0.54$. The energies are renormalized to $E_{J=0} = 0$ in all cases.

	$\langle \Psi^J_{M0}\|H\|\Psi^J_{M0}\rangle$	$\langle \Psi^J_{M0}\|H^{(\mathrm{int})}\|\Psi^J_{M0}\rangle$	$E^{(\mathrm{int})}_J$	E (experimental)	N_J	$N^{(\mathrm{int})}_J$
$J=0$	0.0	0.0	0.0	0.0	0.098	0.099
$J=2$	1.09	1.06	1.08	1.63	0.367	0.371
$J=4$	3.79	3.70	3.77	4.25	0.334	0.335
$J=6$	8.43	8.28	8.39	8.79	0.156	0.154

By doing the angular integrals and using the identity

$$D^{L}_{00}(\Omega)D^{J}_{00}{}^{*}(\Omega) = \sum_{J'} |\langle L0J0|J'0\rangle|^2 D^{J'}_{00}(\Omega), \tag{22}$$

we obtain

$$\langle \Psi^{J}_{M0}| \frac{P^2}{2Am} |\Psi^{J}_{M0}\rangle = N_{J0}{}^{-1} \sum_{L,J'} \frac{2J+1}{2J'+1} E^{\text{c.m.}}_{L} |\langle J'0|L0J0\rangle|^2 N^{(\text{int})}_{J'}, \tag{23}$$

where

$$E^{\text{c.m.}}_{L} = \int_0^\infty F_L(R)\left[\frac{\hbar^2}{2mA}\left(-\frac{1}{R^2}\frac{d}{dR}R^2\frac{d}{dR} + \frac{L(L+1)}{R^2}\right)\right] F_L(R)R^2dR \tag{24}$$

and

$$N^{(\text{int})}_{J'} = \frac{2J'+1}{8\pi^2}\int d\Omega\, D^{J'}_{00}{}^{*}(\Omega)\int d^{3A-3}\vec{\xi}\,\phi^{*(\text{int})}(\vec{\xi})R^{(\text{int})}(\Omega)\phi^{(\text{int})}(\vec{\xi}). \tag{25}$$

We recall that N_{J0} represented the probability that the state $|\phi_0\rangle$ was in an eigenstate of total angular momentum J. The number $N^{(\text{int})}_{J'}$ represents the probability that the intrinsic part of $|\phi_0\rangle$ is in an eigenstate of the intrinsic angular momentum with eigenvalue J' independent of the structure of the center-of-mass part of $|\phi_0\rangle$.

We need only the numbers $E^{\text{c.m.}}_{L}$ and $N^{(\text{int})}_{J'}$ in Eq. (23) to calculate the corrections $\langle\Psi^{J}_{M0}|P^2/2Am|\Psi^{J}_{M0}\rangle$. $E^{\text{c.m.}}_{L}$ is given in terms of simple integrals over the functions $F(\vec{R})$ explicitly exhibited in Eq. (15). The number $N^{(\text{int})}_{J'}$ can be calculated by considering the norm of $|\Psi^{J}_{M0}\rangle$

$$\langle\Psi^{J}_{M0}|\Psi^{J}_{M0}\rangle = N_{J0} = \sum_{J'}\frac{2J+1}{2J'+1}\sum_{L} N^{\text{c.m.}}_{L}|\langle J'0|L0J0\rangle|^2 N^{(\text{int})}_{J'}, \tag{26}$$

with

$$N^{\text{c.m.}}_{L} = \int_0^\infty R^2dR\,|F_L(R)|^2. \tag{27}$$

The derivation of Eq. (26) is identical to the derivation of Eq. (23). As N_{J0} and $N^{\text{c.m.}}_{L}$ are known, Eq. (26) can be inverted to give $N^{(\text{int})}_{J'}$, and hence, through Eq. (23), the corrections to the energy.

The second correction that must be made arises because the physical energies are not correctly given by the expectation value of $H^{(\text{int})}$ with respect to the states $|\Psi^{J}_{M0}\rangle$, as these states are eigenstates of the total (intrinsic plus center-of-mass) angular momentum. The correct eigenstates to use are the eigenstates of the intrinsic angular momentum. These are given by

$$|\phi^{(\text{int})}_{JM}\rangle = (N^{(\text{int})}_{J})^{-1/2}\frac{2J+1}{8\pi^2}\int d\Omega\, D^{J}_{M0}{}^{*}(\Omega)R^{(\text{int})}(\Omega)|\phi^{(\text{int})}\rangle. \tag{28}$$

The correct intrinsic energy is then given by

$$E^{(\text{int})}_{J} = \langle\phi^{(\text{int})}_{JM}|H^{(\text{int})}|\phi^{(\text{int})}_{JM}\rangle = \frac{2J+1}{8\pi^2}(N^{(\text{int})}_{J})^{-1}\int d\Omega\, D^{J}_{00}{}^{*}(\Omega)\langle\phi^{(\text{int})}|H^{(\text{int})}R^{(\text{int})}(\Omega)|\phi^{(\text{int})}\rangle. \tag{29}$$

By using the now familiar algebra, we have for the quantity introduced in Eq. (9),

$$\langle\Psi^{J}_{M0}|H|\Psi^{J}_{M0}\rangle - \langle\Psi^{J}_{M0}|\frac{P^2}{2Am}|\Psi^{J}_{M0}\rangle = \sum_{J'}\frac{2J+1}{2J'+1}\frac{N_{J'}}{N_J}\sum_{L} N^{\text{c.m.}}_{L}|\langle J'0|L0J0\rangle|^2 E^{(\text{int})}_{J'}. \tag{30}$$

This relation may be inverted to give the intrinsic energies $E^{(\text{int})}_{J'}$.

As an example, we have calculated the energies $E^{(\text{int})}_{J'}$ for the projected Hartree-Fock calculation of ^{20}Ne given in Ref. 3. The results are presented in Table I. The corrections to the relative energies are quite small, the maximum being -0.04 MeV for the $J=6$ level. This is because the two corrections made are of the same order of magnitude but of opposite sign and nearly cancel. If a Hartree-Fock calculation is performed using $H^{(\text{int})}$ instead of H, however, then only the second correction is applicable. In this case, we see that the corrections to the relative energies will be of the order of several tenths of an MeV.

To examine this case, we consider the Hartree-Fock calculations of Ripka.[2] In these calculations, however, it is not immediately clear whether the

TABLE II. The harmonic-oscillator parameter $\alpha = (m\omega/\hbar)^{1/2}$, the quadrupole deformation $\mathfrak{D}$, the uncorrected Hartree-Fock energies E_J (Ref. 2), the corrected energies $E_J^{(\mathrm{int})}$, and the experimental energies E_J (exp). All energies have been normalized to $E_{J=0}=0$.

Nucleus	α (fm^{-1})	$\mathfrak{D}$	J	E_J	$E_J^{(\mathrm{int})}$	$E_J^{(\mathrm{exp})}$
^{12}C	0.620	−0.30	2	3.24	3.28	4.43
			4	11.10	11.39	···
^{20}Ne	0.559	0.31	2	1.22	1.23	1.63
			4	3.86	3.89	4.25
			6	7.70	7.78	8.79
			8	11.08	11.23	···
^{28}Si	0.548	−0.30	2	0.70	0.71	1.78
			4	2.30	2.32	4.62
			6	4.76	4.80	···
			8	7.95	8.04	···
^{36}A	0.496	−0.15	2	1.13	1.13	1.98
			4	3.22	3.22	4.1
			6	7.21	7.24	···
			8	10.97	11.03	···

Hamiltonian used is a representation of $H^{(\mathrm{int})}$ or H. As the ^{16}O core is taken to be inert, the Hartree-Fock Hamiltonian takes the form

$$\langle\alpha\,|\,H^{\mathrm{HF}}\,|\,\beta\rangle = \epsilon_\alpha\delta_{\alpha\beta} + \sum_{\mu=1}^{M}\langle\alpha,\mu\,|\,v\,|\,\beta,\mu\rangle - \sum_{\nu=1}^{N}\langle\alpha,\nu\,|\,\beta,\nu\rangle, \tag{31}$$

where ϵ_α is the Hartree-Fock energy of the state α, and the sum over $\mu(\nu)$ is over particles (holes) with ^{16}O taken as a vacuum. Now ϵ_α is replaced by the experimental single-particle energies which are intrinsic quantities. As v is inherently an intrinsic quantity, Eq. (31) must necessarily represent the matrix elements of an intrinsic operator. Thus we consider H^{HF} to be an approximation to $H^{(\mathrm{int})}$, and therefore only the second type of correction, Eq. (30), applies. The corrected energies, $E_J^{(\mathrm{int})}$, were calculated by inverting Eq. (30) for the Hartree-Fock calculations of Ref. 2 for the nuclei ^{12}C, ^{20}Ne, ^{28}Si, and ^{36}Ar. The results are given in Table II. The corrections are seen always to broaden the spacing between levels, with the largest correction being 0.15 MeV for the $J=8$ state of ^{20}Ne.

We thus see that the center-of-mass corrections to the projected Hartree-Fock energies are small, but not negligible. In the case where one uses the total Hamiltonian H, there are two corrections which tend to cancel. In the case of a single major shell calculation, we have identified the Hamiltonian being used with $H^{(\mathrm{int})}$, and have found the corrections to be $\leq$0.15 MeV. The corrections are quite sensitive to the deformation parameter $\mathfrak{D}$. If the restriction to a single major shell is removed, $\mathfrak{D}$ will generally double.[2] A simple extrapolation of our calculations indicates that the center-of-mass correction could become as large as 0.5 MeV. It is thus clear that center-of-mass corrections should be included before a quantitative comparison with experiment can be made.

The center-of-mass corrections made here should not only be applied to the calculation of the energy but to the calculation of any matrix element. We may use Eq. (30) to calculate corrections to the mean value of any intrinsic operator, not just $H^{(\mathrm{int})}$. The extension to off diagonal matrix elements is straightforward.

The authors would like to thank W. F. Ford and R. C. Braley for furnishing certain unpublished numbers from their calculation.

*Supported in part by the National Science Foundation.

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