[2]K. T. R. Davies and R. J. McCarthy, Phys. Rev. C 4, 81 (1971).
[3]A. Kallio and B. D. Day, Nucl. Phys. A124, 177 (1969).
[4]M. Baranger, in *Nuclear Structure and Nuclear Reactions, Proceedings of the International School of Physics "Enrico Fermi," Course XL, Varenna, 1967*, edited by M. Jean and R. A. Ricci (Academic, New York, 1969).
[5]K. T. R. Davies and R. L. Becker, Nucl. Phys. A176, 1 (1971).
[6]We thank Professor M. Baranger for useful suggestions here.
[7]B. H. Brandow, Phys. Rev. 152, 863 (1966); Rev. Mod. Phys. 39, 771 (1967); in *Lectures in Theoretical Physics*, edited by K. T. Mahanthappa and W. E. Brittin (Gordon and Breach, New York, 1969), Vol. XI-B, p. 55; Ann. Phys. (N.Y.) 57, 214 (1970).
[8]R. J. McCarthy and K. T. R. Davies, Phys. Rev. C 1, 1644 (1970).

PHYSICAL REVIEW C VOLUME 7, NUMBER 3 MARCH 1973

Microscopic Theory of Nuclear Collective Motion*

P. K. Haff and L. Wilets
Physics Department, University of Washington, Seattle, Washington 98195
(Received 10 July 1972)

A generalization of the Hill-Wheeler generator coordinate method is applied to collective deformations. The intrinsic wave function is constrained (as in constrained Hartree-Fock) to be characterized not only by a given deformation, but also by a deformation velocity. This is effected by a simple ansatz which involves operation on the singly constrained wave function by an exponentiated single-particle deformation operator containing an arbitrary function $\beta(\alpha)$, where α is the collective variable. The expectation value of the energy is minimized with respect to both $\beta(\alpha)$ and the Hill-Wheeler projection function $f(\alpha)$. This leads to an integral equation for f which, upon invoking the collective nature of the intrinsic states, may be approximated by a second-order differential equation in the deformation coordinate $\alpha = \langle Q \rangle$. In order to reduce this equation to the Schrödinger form, certain assumptions are introduced with regard to the approximate form of f. This procedure leads to two different differential equations for f and to two mass parameters. One is valid in the classical region and one in the classically inaccessible tunneling region. This is to be contrasted to the cranking model where sufficient energy must always be available to drive the system. The expressions for the mass parameter are given in terms of expectation values of few-body operators. The case of uniform translation of the nucleus as a whole is studied in detail. The generalized Hill-Wheeler method as described above produces the correct mass (= total nuclear mass). This rigorous reproduction of a known result allows the study of approximations which become necessary for the general case of deformations. Comments are made about the potential energy of deformation surface, which is expected to lie lower than the expectation value of the Hamiltonian.

I. INTRODUCTION

In the study of collective nuclear motion, the microscopic structure of the nucleus enters the problem by way of the mass parameters and energy surface, which together determine the system dynamics. A purpose of a microscopic theory of collective motion is to determine these parameters explicitly in terms of the nuclear Hamiltonian. Below, we develop expressions for the mass parameter in the form of expectation values of products of the Hamiltonian with other operators. The particular operators which appear depend upon the type of collective motion considered. Primary attention is paid to quadrupole deformation (vibrations and fission) and to translational motion of the nucleus as a whole.

This latter motion is interesting for two reasons: First, the correct mass (which is the total nuclear mass mA) is given incorrectly by the simple projection method[1-4] to be discussed below. It would be reassuring for such a microscopic theory to give the correct result, although that in itself would not guarantee the validity of the theory for other collective motions of the nucleus. We introduce a modification of the projection method which will yield the mass mA.

Second, if a formalism produces the correct mass in the translational case, it may be possible to use this knowledge as a check on approximations which are necessary in the study of other types of collective motion. The translational case is discussed in detail in Sec. III.

The present approach is particularly interesting

due to the variational way in which the collective velocity is treated and to the subsequent choice that we find for the inertia parameter. Depending upon whether the system is in a classical or a tunneling region of deformation, different forms of the mass obtain. The details of the development are given in Sec. II, before proceeding to applications to translational motion.

In the remainder of the Introduction, we will very briefly sketch some microscopic theories of collective motion, particularly the cranking[5] and projection[1-4] approaches, in order to put our formalism into perspective. Detailed discussions of these theories of collective motion have been given, for example, in the lectures of Klein[6] and Villars,[7] and by Brink and Weiguny,[8] and by Wong.[9]

In the cranking model, as it was first applied to rotations,[5] the nucleons are placed in a deformed potential well which is then externally and slowly rotated (slowly so that the particle orbits adjust quasiadiabatically to the changing well orientation). The energy increase due to rotation is evaluated in perturbation theory, and equated to $\frac{1}{2}\mathcal{I}\omega^2$. Here $\mathcal{I}$ is the moment of inertia and ω the angular velocity with which the well is driven.

In this way the following expression for the moment of inertia for rotation about the x axis is obtained, in first-order perturbation theory,

$$\mathcal{I}_{\text{cranking}} = 2\hbar^2 \sum_{n\neq 0} \frac{|\langle n|J_x|0\rangle|^2}{E_n - E_0}. \tag{1}$$

The bras and kets refer to states of a model single-particle Hamiltonian, $n=0$ representing the ground state, and the E_n are the corresponding energies. J_x is the x component of the total angular momentum operator. For the case where the wave functions $|n\rangle$ are composed of independent-particle orbitals, the cranking formula (1) gives just the rigid-body moment of inertia.[5]

A similar approach may be followed in deriving a formula to express the mass parameter for vibrations. Again we specialize to the adiabatic assumption that the collective motion is much slower than the particle motion. A set of parameters describing the nuclear deformation may be denoted by α, and these are considered to be prescribed functions of the time, $\alpha = \alpha(t)$. The solution of the time-dependent Schrödinger equation through first order in $\dot{\alpha}$ for the wave function leads to the energy

$$E = E_0 + \tfrac{1}{2}B\dot{\alpha}^2, \tag{2}$$

where

$$B = B_{\text{cranking}} = 2\hbar^2 \sum_{k\neq 0} \frac{|\langle k|\partial/\partial\alpha|0\rangle|^2}{E_k - E_0}. \tag{3}$$

It is of interest to note a refinement to the simple cranking model which introduces constraints in a manner we shall find useful in Sec. II. This is the "self-consistent" cranking model, associated with Thouless and Valatin.[10,11]

In this approach, one uses Hartree-Fock theory and minimizes the total energy subject to the constraint that the angular momentum about the rotation axis have a fixed average value. If the rotation axis is the x axis, then the constraint is included by minimizing

$$H - \omega J_x, \tag{4}$$

where ω is a Lagrange multiplier, to be interpreted as an angular velocity. The moment of inertia is deduced from the equation

$$\langle\phi|J_x|\phi\rangle = \frac{\mathcal{I}\omega}{\hbar}, \tag{5}$$

where $|\phi\rangle$ is the Hartree-Fock solution generated from (4). The moment of inertia is given by the expression

$$\mathcal{I}_{TV} = \frac{\hbar}{\omega}\sum_{\text{ph}}(\langle p|J_x|h\rangle C^*_{\text{ph}} + \langle h|J_x|p\rangle C_{\text{ph}}), \tag{6}$$

where p and h refer to particle and hole states, respectively. The coefficients C_{ph} are in turn defined by

$$(\epsilon_p - \epsilon_h)C_{\text{ph}} + \sum_{p'h'}(\langle ph'|V|hp'\rangle C_{p'h'} + \langle pp'|V|hh'\rangle C_{p'h'}) = \hbar\omega\langle p|J_x|h\rangle, \tag{7}$$

where ϵ_p and ϵ_h are particle and hole energies, and V is the antisymmetrized two-body interaction. In general then, a matrix inversion is necessary to find $\mathcal{I}_{TV}$. Neglecting the interaction, (6) leads back to the cranking form

$$\mathcal{I}_{TV} \xrightarrow[V\to 0]{} 2\hbar^2 \sum_{\text{ph}} \frac{|\langle p|J_x|h\rangle|^2}{\epsilon_p - \epsilon_h}. \tag{8}$$

The Thouless-Valatin or "self-consistent cranking" formula, Eq. (6), like the cranking formula itself, is semiclassical.

One may go beyond the semiclassical approaches outlined above by appealing to the projection methods. These are specializations of the Hill-Wheeler method of generator coordinates.[1,2] (For a discussion of the relationship of the generator coordinate approach to the cranking approach, see the recent lectures by Klein.[6]) In the projection method, one first labels the intrinsic wave function $\phi(\vec{r}_i \cdots \vec{r}_A) \equiv \phi(\vec{r})$ by a parameter(s) α specifying some collective property associated with ϕ. Thus α might be the Euler angles specifying the orientation of a deformed Hartree-Fock determinant with respect to a space-fixed axis, or a deformation parameter

specifying (perhaps equal to) the nuclear quadrupole moment $\langle\phi|Q_{20}|\phi\rangle$. A trial wave function to be used in energy minimization is constructed by integrating over α,

$$\psi(\vec{\mathbf{r}}) \equiv \int d\alpha f(\alpha)\phi(\vec{\mathbf{r}}, \alpha). \tag{9}$$

The weighting function f, which is to be interpreted as the collective wave function in the variable α, is determined from the variational equation

$$\delta \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0, \tag{10}$$

where the angular brackets indicate both spatial and α integration.

In the Peierls-Yoccoz theory of the moment of inertia,[3] α is taken to be the three Euler angles of rotation, Ω,

$$\alpha \equiv \Omega = (\theta_1, \theta_2, \theta_3). \tag{11}$$

If $\phi(\vec{\mathbf{r}})$ has its symmetry axis along the space-fixed z axis, then the prescription

$$\phi(\vec{\mathbf{r}}, \Omega) = R(\Omega)\phi(\vec{\mathbf{r}}), \tag{12}$$

where R is the rotation operator

$$R = e^{-i\theta_1 J_z} e^{-i\theta_2 J_y} e^{-i\theta_3 J_z}, \tag{13}$$

is one way we may label ϕ by the variables Ω. From Eq. (10), using Eq. (12), we find

$$f(\Omega) = \mathfrak{D}^J_{MK}(\Omega). \tag{14}$$

The operation (9) then projects out the component of ϕ with angular momentum J. By computing the total energy

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = E_0 + \frac{1}{2\mathcal{I}_{\mathrm{PY}}} J(J+1), \tag{15}$$

the Peierls-Yoccoz moment of inertia may be determined,

$$\mathcal{I}_{\mathrm{PY}} = \frac{|\langle J_x^2\rangle|^2}{\langle H J_x^2\rangle - \langle H\rangle\langle J_x^2\rangle}. \tag{16}$$

This result is for rotation about the x axis. When the same approach is applied to translation of the nucleus as a whole, the generator coordinate may be identified with the displacement Z of the center of mass. Then

$$\Psi(\vec{\mathbf{r}}) = \int dZ f(Z)\phi(\vec{\mathbf{r}}, Z) = \int dZ f(Z)\phi(\vec{\mathbf{r}}_{\mathrm{int}}; R - Z), \tag{17}$$

where R is the z component of the center-of-mass coordinate and $\vec{\mathbf{r}}_{\mathrm{int}}$ are internal coordinates. We specialize to one-dimensional center-of-mass motion for simplicity. Then, following Eq. (12),

$$\phi(\vec{\mathbf{r}}, Z) = e^{-iPZ}\phi(\vec{\mathbf{r}}), \tag{18}$$

where P is the z component of the center-of-mass momentum operator. In this case symmetry leads to the equation

$$f(Z) = e^{ikZ} \tag{19}$$

and computation of the total energy

$$E = E_0 + \frac{1}{2M_{\mathrm{PY}}} k^2 + \cdots \tag{20}$$

yields the Peierls-Yoccoz mass

$$M_{\mathrm{PY}} = \frac{|\langle P^2\rangle|^2}{\langle H P^2\rangle - \langle H\rangle\langle P^2\rangle}$$

which in general is not equal to the total mass.[2,4] This is a defect we wish to avoid. Not only is it displeasing to produce the incorrect result in this simple case, but the failure casts doubt upon the rotational result Eq. (16). The difficulty may be traced to the form used for the intrinsic wave function (18). A more general wave function is needed. (The translational case is discussed in detail in Sec. III.)

An attempt to produce the correct translational mass, still remaining within the framework of the projection method, is the double projection method of Peierls and Thouless.[4] They noted that the Peierls-Yoccoz wave function

$$\Psi_k(\vec{\mathbf{r}}_{\mathrm{int}}; R) = \int dZ\, e^{ikZ}\phi(\vec{\mathbf{r}}_{\mathrm{int}}; R - Z) \tag{21}$$

is not Galilean invariant. That is

$$\Psi_k(\vec{\mathbf{r}}_{\mathrm{int}}; R) = e^{ikR}\psi(k; \vec{\mathbf{r}}_{\mathrm{int}}), \tag{22}$$

where ψ depends not only on the intrinsic coordinates but also on the momentum k, because a different function of relative coordinates is projected out for each k. For Galilean invariance, ψ must be independent of k.

To accomplish this a wave function may be generated which has a mean center-of-mass momentum $\langle P\rangle$. Using constrained Hartree-Fock theory (for example), the Hamiltonian

$$H - vP \tag{23}$$

is minimized with respect to a trial wave function. This procedure yields the function

$$\phi_v(\vec{\mathbf{r}}_{\mathrm{int}}; R) = e^{iMvR}\phi_0(\vec{\mathbf{r}}_{\mathrm{int}}; R), \tag{24}$$

where M is the nuclear mass, and v is a Lagrange multiplier with the dimensions of a velocity. Different choices of the parameter v correspond to different choices of mean momentum $\langle P\rangle$. Translating the solution (24) an amount Z gives a two-

parameter wave function $\phi_v(\vec{r}_{\rm int}; R-Z)$. Since the center-of-mass motion should leave the internal structure unaffected, it is reasonable to take a linear combination of the wave functions $\phi_v(\vec{r}_{\rm int}; R-Z)$, for different v, as well as to project out a component of linear momentum. Thus we have

$$\Psi_k(\vec{r}) = \iint dv dZ\, g_k(v) e^{ikZ} \phi_v(\vec{r}_{\rm int}; R-Z)\,. \tag{25}$$

If v is chosen to be related to k by

$$Mv = k - k'\,,$$

then

$$\Psi_k(\vec{r}) = e^{ikR} \iint dk' dZ\, g_k(k') e^{-ik'(R-Z)} \phi_0(\vec{r}_{\rm int}; R-Z) \tag{26}$$

has center-of-mass momentum k. The choice

$$g_k(k') \equiv \delta(k-k') \tag{27}$$

leads back to the Peierls-Yoccoz result, Eq. (21). If $g_k(k')$ is independent of k, however, then the wave function Ψ_k is Galilean invariant since it is a function of the intrinsic coordinates only, multiplied by $\exp(ikR)$. In principle g is determined variationally, although such a procedure is very cumbersome even for translational motion.

The formal results which we find below, when applied to translations in Sec. III, essentially reduce to the form (26) with the special choice

$$g_k(k') \equiv g(k') = \delta(k')\,, \tag{28}$$

so that we have the simple result

$$\Psi_k = e^{ikR} \int dZ\, \phi(\vec{r}_{\rm int}; Z)\,. \tag{29}$$

A recent treatment of this problem by Villars and Schmeing-Rogerson[12] does produce the correct translational mass. Although it does not address the vibrational problem, it exhibits sufficient similarity to our approach to warrant discussion. The idea is to endow the intrinsic wave function ϕ_0 (a Hartree-Fock determinant) with a greater generality in the manner

$$\phi_0 \to \phi = e^{iF} \phi_0\,, \tag{30}$$

where F is a single-particle operator. The "best" operator F is then determined by variation of the expectation value of the Hamiltonian with respect to the projected wave function

$$\Psi = \int dZ\, e^{ikZ} e^{-iPZ} e^{iF} \phi_0(\vec{r})\,, \tag{31}$$

where P is the center-of-mass momentum operator. This same approach of "variation after projection," first discussed by Rouhaninejad and Yoccoz,[13] is also applied by them to the moment-of-inertia problem.

In our formalism, discussed in Secs. II and III below, we make a simpler ansatz than Eq. (30). The form of F is not left completely general. A restricted set of forms is chosen, dictated by the particular collective motion of interest, and the best F is variationally determined from among the members of the set. For translations it turns out (Sec. III) that a reasonable form for F is

$$F = \beta(Z) R\,, \tag{32}$$

where R is the center-of-mass coordinate and $\beta(Z)$, a function of the collective coordinate Z and not a particle operator, is to be chosen to minimize the energy. Then we find

$$\beta = k\,, \tag{33}$$

a constant, so that Eq. (31) becomes

$$\Psi \to \Psi_k = \int dZ\, e^{ikZ} e^{ik(R-Z)} \phi_0(\vec{r}_{\rm int}; R-Z)\,, \tag{34}$$

or

$$\Psi_k = e^{ikR} \int dZ\, \phi_0(\vec{r}_{\rm int}; Z)\,, \tag{35}$$

which is the same as Eq. (29) and gives the correct translational motion.

In addition to translational and rotational motion, the generator coordinate method has been applied to clustering phenomena in nuclei[8,14] and to nuclear scattering.[15]

In Sec. II we develop the general formula for the mass parameter B, keeping in mind the case of vibrations or fission. The formulation is general, however, and in Sec. III uniform translational motion is studied in detail. Finally, in Sec. IV the general mass parameter expression of Sec. II is reduced to tractable form for vibrations (fission) under suitable assumptions.

II. FORMAL DEVELOPMENTS

The approach of the present paper is to derive a second-order differential equation for the collective wave function $f(\alpha)$ of the form

$$-\frac{d}{d\alpha}\frac{1}{2B(\alpha)}\frac{d}{d\alpha} f(\alpha) + [V(\alpha) - E] f(\alpha) = 0 \tag{36}$$

in which the mass parameter $B(\alpha)$ may be identified. Here α is an appropriate collective coordinate, $V(\alpha)$ is the potential energy, and E is the total energy. We proceed by generating an intrinsic wave function which contains in it the proper collective motion (using constrained Hartree-Fock theory,[7,16] for example), and then projecting with the collective wave function $f(\alpha)$ in the manner of Hill and Wheeler.[1,2] An equation for the wave func-

tion f, which may be reduced to the form (36), is determined from a variational principle.

A. Intrinsic Wave Function

In order to obtain the energy or wave function for arbitrary deformation, the energy minimization is subjected to the constraint that (say) the quadrupole moment operator

$$Q=\sum_{i=1}^{A} q_i$$

have a prescribed expectation value. This is equivalent to minimizing the expectation value of

$$\hat{H}=H+\tilde{\alpha}Q\,, \tag{37}$$

where $\tilde{\alpha}$ is a Lagrange multiplier and the term $\tilde{\alpha}Q$ acts like an externally applied (single-particle) potential.

The corresponding intrinsic A-body wave function is $\hat{\psi}(\vec{r}_1,\ldots,\vec{r}_A;\alpha)$. Here α is a parameter which labels the deformation of the wave function. For example, α may be taken to be the Lagrange multiplier $\tilde{\alpha}$, or the quadrupole moment $\langle Q\rangle$. This latter choice will generally be convenient.

Although this technique makes it possible to produce wave functions of arbitrary quadrupole moment,[17] the dynamics of collective motion are not explicitly included. The intrinsic wave function should also reflect collective motion. This suggests that not only the value of the deformation $\langle Q\rangle$ but also of $\langle\dot{Q}\rangle$ should be specified for the intrinsic wave function. These requirements are met by minimization of the expectation value of the generator Hamiltonian

$$\tilde{H}=H+\tilde{\alpha}Q-\beta\dot{Q}\,. \tag{38}$$

A discussion of Hamiltonians such as in Eq. (38) from the point of view of Hartree-Fock theory may be found in the lectures by Villars.[7]

The A-body wave function $\tilde{\psi}(\vec{r},\alpha,\beta)$ is then labeled by both α and β. The quantity β is taken to be a function of $\alpha=\langle Q\rangle$ and its precise form is to be determined by variation of the total energy. A nonzero value of β should lead to a nonzero collective velocity. The variational determination of β is then essentially a self-consistent cranking approach. The assumption $\beta=\beta(\alpha)$ means that the velocity depends only upon the local deformation, rather than upon all deformations. Such an assumption avoids the calculational difficulties attendant upon a double projection formulation.[4]

In Hartree-Fock the determinant minimizing Eq. (38) may be written, for small β, as[16]

$$\tilde{\psi}(\vec{r},\alpha,\beta)=e^{i\Lambda}\hat{\psi}(\vec{r},\alpha)\,, \tag{39}$$

where $\hat{\psi}$ is a determinant of Hartree-Fock functions generated by $H+\tilde{\alpha}Q$ and Λ is a single-particle operator which satisfies

$$i(\mathrm{ph}|[H,\Lambda]|0)=\beta(\mathrm{ph}|\dot{Q}|0)\,. \tag{40}$$

Here $|0)$ refers to $\hat{\psi}(\vec{r},\alpha)$ and $|\mathrm{ph})$ to a particle-hole state built upon $|0)$.

A solution to Eq. (40) is

$$\Lambda=\beta[Q-g(\alpha)]\,, \tag{41}$$

where $g(\alpha)$ is a c number specifying a deformation-dependent phase for the function (39). In the absence of the Hartree-Fock approximation, the form (39) may be obtained through conventional perturbation theory. Thus

$$\tilde{\psi}(\vec{r},\alpha,\beta(\alpha))=e^{i\beta(\alpha)[Q-g(\alpha)]}\hat{\psi}(\vec{r},\alpha)\,. \tag{42}$$

Equation (42) will be our ansatz for the intrinsic wave function for all β. The actual form of g is chosen to obtain a convenient interpretation of $f(\alpha)$. Below, in Sec. II C, β is shown to have the form

$$\beta(\alpha)=A+B_2\frac{f'}{f}+B_1\frac{f^{*\prime}}{f^*}\,, \tag{43}$$

where A, B_1, and B_2 depend upon g and α. In general, A is nonzero, so Eq. (43) implies that even when the collective velocity vanishes, as indicated by the wave-function behavior $f'/f\to 0$, the generating term $\beta\dot{Q}$ continues to enforce a collective motion upon the system. However, if g is determined from the equation

$$A(\alpha,g(\alpha))=0\,, \tag{44}$$

then β will be proportional to the "velocity," which is the behavior we desire. The explicit form for the function g is given below.

The following points are important:

(a) The Lagrange multiplier $\tilde{\alpha}$ is real in order that $\hat{H}$ be Hermitian, since Q is Hermitian.

(b) We choose $\hat{\psi}$ to be real, in which case $\tilde{\psi}$ will generally be complex.

(c) Although we have chosen β to be a function of α, it will be determined variationally. This will produce the best β consistent with such a restriction.

B. Projected Wave Function and the Total Energy

The A-body wave function is generated by the Hill-Wheeler projection technique,[1,2]

$$\begin{aligned}\Psi(\vec{r}_1,\ldots,\vec{r}_A)&\equiv\int d\alpha f(\alpha)\tilde{\psi}(\vec{r}_1,\ldots,\vec{r}_A;\alpha,\beta(\alpha))\\&=\int d\alpha f(\alpha)e^{i\beta(\alpha)[Q-g(\alpha)]}\hat{\psi}(\vec{r},\alpha)\,.\end{aligned} \tag{45}$$

Note that a change of the form of g corresponds to a change in the definition of the collective wave function f. With the choice dictated by Eq. (44) the motion associated with the intrinsic function is generated in a physically reasonable manner so that f is a suitable collective wave function.

With Eq. (45) as a complex trial wave function the energy $\langle\Psi|H|\Psi\rangle$ is minimized subject to the condition that $\langle\Psi|\Psi\rangle = 1$. This leads to

$$\delta\langle\Psi|H-E|\Psi\rangle = 0\,, \tag{46}$$

where the energy E is, in fact, a Lagrange multiplier for the normalization. The expectation value is to be varied simultaneously with respect to both $\beta(\alpha)$ and $f(\alpha)$. Substituting the form (45) into Eq. (46) and defining $H - E \equiv \overline{H}$ we obtain the expectation value

$$\langle\Psi|\overline{H}|\Psi\rangle = \iint d\alpha d\alpha' \int d\vec{\mathbf{r}} f^*(\alpha) f(\alpha') \tilde{\psi}^*(\vec{\mathbf{r}}, \alpha, \beta(\alpha)) \overline{H} \tilde{\psi}(\vec{\mathbf{r}}, \alpha', \beta(\alpha'))\,. \tag{47}$$

In terms of the functions $\hat{\psi}$, Eq. (47) may be written

$$\langle\Psi|\overline{H}|\Psi\rangle = \iint d\alpha d\alpha' f^*(\alpha) f(\alpha') \int d\vec{\mathbf{r}}\, e^{-i\beta^*(\alpha)\overline{Q}(\vec{\mathbf{r}},\alpha)} \hat{\psi}^*(\vec{\mathbf{r}}, \alpha) \overline{H} e^{i\beta(\alpha')\overline{Q}(\vec{\mathbf{r}},\alpha')} \hat{\psi}(\vec{\mathbf{r}}, \alpha')\,. \tag{48}$$

In the above expression

$$\overline{Q}(\vec{\mathbf{r}}, \alpha) \equiv Q(\vec{\mathbf{r}}) - g(\alpha)\,. \tag{49}$$

In Eq. (48) g has been chosen to be real. The condition (44) may still be satisfied.

To make further progress we expand the exponential factors in Eq. (48), keeping terms through order β^2 (i.e., through order f'^2/f). As shown below, terms of this order are necessary in order to compute correctly the mass parameter (= total nuclear mass) for translation of the nucleus as a whole. With some new notation Eq. (48) becomes

$$\begin{aligned}\langle\Psi|\overline{H}|\Psi\rangle = \iint d\alpha d\alpha' f^*(\alpha) f(\alpha') [&(\alpha|\overline{H}|\alpha') - i\beta^*(\alpha)(\alpha|\overline{Q}\overline{H}|\alpha') + i\beta(\alpha')(\alpha|\overline{H}\overline{Q}|\alpha') \\ &- \tfrac{1}{2}\beta^{*2}(\alpha)(\alpha|\overline{Q}^2\overline{H}|\alpha') - \tfrac{1}{2}\beta^2(\alpha')(\alpha|\overline{H}\overline{Q}^2|\alpha') + \beta^*(\alpha)\beta(\alpha')(\alpha|\overline{Q}\overline{H}\overline{Q}|\alpha')]\,.\end{aligned} \tag{50}$$

The functions $\hat{\psi}(\vec{\mathbf{r}}, \alpha)$ are represented by the appropriate rounded bra and ket notation, with bra-kets integrated over $\vec{\mathbf{r}}$. The operators $\overline{Q}$ and $\overline{Q}^2$ are understood to be functions of the variable (α or α') of the adjoining bra or ket, e.g.,

$$(\alpha|\overline{Q}\overline{H}\overline{Q}|\alpha') \equiv (\alpha|\overline{Q}(\alpha)\overline{H}\overline{Q}(\alpha')|\alpha')\,.$$

C. Energy Minimization and the Differential Equation

Varying Eq. (50) with respect to β^* and setting the result equal to zero,

$$\frac{\delta}{\delta\beta^*(\alpha)}\langle\Psi|\overline{H}|\Psi\rangle = 0\,,$$

yields, to order β, the integral equation

$$\int d\alpha' f(\alpha')[(\alpha|\overline{Q}\overline{H}|\alpha') - i\beta^*(\alpha)(\alpha|\overline{Q}^2\overline{H}|\alpha') + i\beta(\alpha')(\alpha|\overline{Q}\overline{H}\overline{Q}|\alpha')] = 0\,. \tag{51a}$$

Similarly, variation with respect to β

$$\frac{\delta}{\delta\beta(\alpha')}\langle\Psi|\overline{H}|\Psi\rangle = 0$$

yields

$$\int d\alpha f^*(\alpha)[(\alpha|\overline{H}\overline{Q}|\alpha') + i\beta(\alpha')(\alpha|\overline{H}\overline{Q}^2|\alpha') - i\beta^*(\alpha)(\alpha|\overline{Q}\overline{H}\overline{Q}|\alpha')] = 0\,. \tag{51b}$$

Equations (51) may be used to simplify the expression for the total energy, Eq. (50). Multiply Eq. (51a) by $[-i\beta^*(\alpha)f(\alpha)/2]$, integrate over α, and subtract from Eq. (50). If Eq. (51b) is used in an analogous fashion, the energy (50) becomes

$$\langle\Psi|\overline{H}|\Psi\rangle = \iint d\alpha d\alpha' f^*(\alpha) f(\alpha')[(\alpha|\overline{H}|\alpha') - \tfrac{1}{2}i\beta^*(\alpha)(\alpha|\overline{Q}\overline{H}|\alpha') + \tfrac{1}{2}i\beta(\alpha')(\alpha|\overline{H}\overline{Q}|\alpha')]\,. \tag{52}$$

The integral Eqs. (51) are more compactly written as

$$0=\{\overline{Q}\overline{H}f\}-i\beta^*(\alpha)\{\overline{Q}^2\overline{H}f\}+i\{\overline{Q}\overline{H}\overline{Q}f\beta\}, \tag{53a}$$

$$0=\{\overline{Q}\overline{H}f^*\}+i\beta(\alpha)\{\overline{Q}^2\overline{H}f^*\}-i\{\overline{Q}\overline{H}\overline{Q}f^*\beta^*\}. \tag{53b}$$

The curly bracket symbols are functions of α and are defined as

$$\{\mathcal{O}\}\equiv\frac{\int d\alpha'(\alpha|\mathcal{O}|\alpha')}{N(\alpha)}, \tag{54}$$

where

$$N(\alpha)\equiv\int d\alpha'(\alpha|\alpha'). \tag{55}$$

For example,

$$\{\overline{Q}\overline{H}f\}=\frac{\int d\alpha' f(\alpha')(\alpha|\overline{Q}(\alpha)\overline{H}|\alpha')}{N(\alpha)}.$$

The derivation of Eqs. (53) from Eqs. (51) made use of the fact that

$$(\alpha|\overline{H}\overline{Q}^n|\alpha')=(\alpha'|\overline{Q}^n\overline{H}|\alpha), \tag{56}$$

where n is a positive integer, and

$$(\alpha|\overline{Q}\overline{H}\overline{Q}|\alpha')=(\alpha'|\overline{Q}\overline{H}\overline{Q}|\alpha). \tag{57}$$

Equation (53b) is the complex conjugate of (53a).

We wish to solve Eqs. (53) for $\beta(\alpha)$ in terms of $f(\alpha)$, substitute the resulting expression into the total energy Eq. (52), and then finally minimize again with respect to f. To solve Eq. (53) it is assumed that, for a fixed value of α, the range of α' over which there are important contributions to the integral $\{\overline{Q}\overline{H}\overline{Q}f\beta\}=\int d\alpha' f(\alpha')\beta(\alpha')(\alpha|\overline{Q}\overline{H}\overline{Q}|\alpha')/N(\alpha)$ is restricted to a small neighborhood of $\alpha'=\alpha$. That is, the matrix element $(\alpha|\overline{Q}\overline{H}\overline{Q}|\alpha')$ is supposed to be sufficiently sharply peaked about $\alpha'=\alpha$ that

$$\{\overline{Q}\overline{H}\overline{Q}f\beta\}\approx\beta(\alpha)\{\overline{Q}\overline{H}\overline{Q}f\} \tag{58}$$

is a good approximation. (Such approximations are discussed below.)

If Eq. (58) is valid, then Eqs. (53) become two simultaneous algebraic equations for β and β^* which may be solved to give

$$\beta(\alpha)=i\frac{[\{\overline{Q}\overline{H}\overline{Q}f^*\}\{\overline{Q}\overline{H}f\}-\{\overline{Q}^2\overline{H}f\}\{\overline{Q}\overline{H}f^*\}]}{|\{\overline{Q}\overline{H}\overline{Q}f\}|^2-|\{\overline{Q}^2\overline{H}f\}|^2}. \tag{59}$$

Since we wish to compute the energy through terms proportional to f'^2 or f'' [to arrive at an equation such as Eq. (36)], it is sufficient to evaluate β, which generates corrections to the wave function $\hat{\psi}$, only through terms proportional to f'. If it is assumed that all matrix elements $(\alpha|\mathcal{O}|\alpha')$ are strongly peaked about $\alpha'=\alpha$ and the first two terms in the Taylor expansion of f are kept, then β becomes

$$\beta(\alpha)\approx i\Big[\{\overline{Q}\overline{H}\}(\{\overline{Q}\overline{H}\overline{Q}\}-\{\overline{Q}^2\overline{H}\})+\frac{f^{*\prime}(\alpha)}{f^*(\alpha)}(\{\overline{Q}\overline{H}\overline{Q}\}_1\{\overline{Q}\overline{H}\}-\{\overline{Q}^2\overline{H}\}\{\overline{Q}\overline{H}\}_1)$$
$$+\frac{f'(\alpha)}{f(\alpha)}(\{\overline{Q}\overline{H}\overline{Q}\}\{\overline{Q}\overline{H}\}_1-\{\overline{Q}^2\overline{H}\}_1\{\overline{Q}\overline{H}\})\Big]\Big/[|\{\overline{Q}\overline{H}\overline{Q}\}|^2-|\{\overline{Q}^2\overline{H}\}|^2]. \tag{60}$$

The curly bracket notation has been generalized such that

$$\{\mathcal{O}\}_n\equiv\int d\alpha'(\alpha|\mathcal{O}|\alpha')(\alpha'-\alpha)^n/N(\alpha) \tag{61a}$$

and

$$\{\mathcal{O}\}_0\equiv\{\mathcal{O}\}. \tag{61b}$$

Choosing $g(\alpha)$ according to the condition (44) so that β, Eq. (60), is proportional to the velocity, we find

$$g(\alpha)=\frac{\{Q\overline{H}\}}{\{\overline{H}\}}, \tag{62}$$

a real function of α. β then has the form

$$\beta(\alpha) = i\frac{\{\overline{QH}\}_1}{\{\overline{QHQ}\}^2 - \{\overline{Q^2H}\}^2}\left[\frac{f'(\alpha)}{f(\alpha)}\{\overline{QHQ}\} - \frac{f'^*(\alpha)}{f^*(\alpha)}\{\overline{Q^2H}\}\right]$$
$$\equiv i\left[B_2(\alpha)\frac{f'(\alpha)}{f(\alpha)} + B_1(\alpha)\frac{f'^*(\alpha)}{f^*(\alpha)}\right]. \tag{63}$$

When expression (63) for β is substituted into the total energy, Eq. (52), the result is

$$\langle\Psi|\overline{H}|\Psi\rangle = \iint d\alpha d\alpha' \Big\{ f^*(\alpha)f(\alpha')\Big[(\alpha|\overline{H}|\alpha') - \frac{1}{2}\frac{f'(\alpha)}{f(\alpha)}B_1(\alpha)(\alpha|\overline{QH}|\alpha') - \frac{1}{2}\frac{f'^*(\alpha')}{f^*(\alpha')}B_1(\alpha')(\alpha|\overline{HQ}|\alpha')\Big]$$
$$- \tfrac{1}{2}f(\alpha')f'^*(\alpha)B_2(\alpha)(\alpha|\overline{QH}|\alpha') - \tfrac{1}{2}f^*(\alpha)f'(\alpha')B_2(\alpha')(\alpha|\overline{HQ}|\alpha')\Big\}. \tag{64}$$

The form of the equation ultimately desired for the collective wave function f is

$$-\frac{d}{d\alpha}\frac{1}{2B(\alpha)}\frac{d}{d\alpha}f(\alpha) + [V(\alpha) - E]f(\alpha) = 0. \tag{65}$$

This suggests that prior to minimization Eq. (64) be cast into the form

$$\langle\Psi|\overline{H}|\Psi\rangle = \int d\alpha f^*(\alpha)\left\{-\frac{d}{d\alpha}\frac{1}{2B(\alpha)}\frac{d}{d\alpha} + [V(\alpha) - E]\right\}f(\alpha) = 0. \tag{66}$$

Such a program may be carried out with the assumption, used above, that the spatial matrix elements are peaked at $\alpha' = \alpha$. Consider the terms containing B_2. By switching variables in the final term and making use of Eq. (56) these terms may be written as

$$-\frac{1}{2}\iint d\alpha d\alpha'[f(\alpha')f'^*(\alpha) + f^*(\alpha')f'(\alpha)]B_2(\alpha)(\alpha|\overline{QH}|\alpha').$$

Expanding $f(\alpha')$ and $f^*(\alpha')$ about $\alpha' = \alpha$ and retaining only terms proportional to the second, or lower, derivatives of f (use of peaked nature of matrix elements) there results

$$-\frac{1}{2}\iint d\alpha d\alpha'\Big([f(\alpha)f'^*(\alpha) + f^*(\alpha)f'(\alpha)]$$
$$+[f'(\alpha)f'^*(\alpha) + f'^*(\alpha)f'(\alpha)](\alpha' - \alpha)\Big)B_2(\alpha)(\alpha|\overline{QH}|\alpha'). \tag{67}$$

Integration by parts yields

$$\int d\alpha f^*(\alpha)\int d\alpha'\left(\frac{d}{d\alpha}[B_2(\alpha)(\alpha|\overline{QH}|\alpha')(\alpha' - \alpha)]\frac{d}{d\alpha}f(\alpha) + \tfrac{1}{2}f(\alpha)\frac{d}{d\alpha}[B_2(\alpha)(\alpha|\overline{QH}|\alpha')]\right), \tag{68}$$

which is of the desired form (66).

The transformation of the terms containing B_1, proceeds initially in the same way. However, the following expression appears:

$$\int d\alpha\int d\alpha'\left(\frac{f^*(\alpha)f'^2(\alpha)}{f(\alpha)} + \frac{f(\alpha)f'^{*2}(\alpha)}{f^*(\alpha)}\right)h(\alpha,\alpha'), \tag{69}$$

which cannot be manipulated by the above procedures to look like Eq. (66). Here $h(\alpha,\alpha')$ is a function of α and α' and involves B_1. The expression (69) may be simplified in an approximate manner by the following considerations. If the potential energy surface is slowly varying with respect to the local "wavelength" $2\pi/k$ associated with the deformation velocity, then in the spirit of the cranking model, f is expected to have the following behavior

$$f_1 \propto e^{\pm ik_1\alpha}, \quad E > V(\alpha) \tag{70a}$$

for a real velocity, or

$$f_2 \propto e^{\pm k_2\alpha}, \quad E < V(\alpha) \tag{70b}$$

for an imaginary velocity. $V(\alpha)$ is the potential energy. In the classical region we consequently make the approximate identification

$$\frac{f^*f'^2}{f} \to -f'^*f', \tag{71a}$$

while in the tunneling region

$$\frac{f^*f'^2}{f} \to +f'^*f'. \tag{71b}$$

[*Note added in proof:* It might be argued that in the classical region ($E > V$) we could also choose

f to be a standing wave, and hence real, in which case (71b) would also obtain. This, however, would destroy the physical content of the flow associated with $\tilde{\psi}$. Rather, we make the semiclassical approximation (70a) and replace (for standing waves) $\Psi \to \Psi + \Psi^*$. Neglect of cross terms between Ψ and Ψ^* in the energy leads to the same result as for the traveling wave case.]

With Eqs. (71), the expression (69) has, upon integration by parts, the required form (66). There now exists a pair of distinct differential equations for f, and hence a pair of mass parameter formulas, each appropriate to the regions of deformation specified by the energy conditions in Eqs. (70). In the vicinity of the transition point between the regions of validity of Eqs. (70a) and (70b), where the particular forms given for f are no longer expected to hold, the curvature of the wave function approaches zero, and consequently the value of the mass parameter is unimportant. As a final point it may be noted that the forms (61) leading to two distinct equations for f affect only the kinetic energy terms, so that only one form for the potential energy will be generated.

With Eqs. (70) the expression (69) is equivalent to

$$\mp 2 \iint d\alpha d\alpha' f^{*\prime}(\alpha) f'(\alpha) h(\alpha, \alpha'), \tag{72}$$

where the upper sign corresponds to the choice (70a) and the lower one to (70b) (this convention to be followed below), or

$$\pm 2 \int d\alpha f^*(\alpha) \int d\alpha' \frac{d}{d\alpha} h(\alpha,\alpha') \frac{d}{d\alpha} f(\alpha). \tag{73}$$

Note that the ansatz (70a) is correct for the translational case. In that case, as discussed in detail in Sec. III, the collective wave function f is just e^{ikz}, where k is the center-of-mass momentum of the nucleus and Z is the parameter (corresponding to α) which describes the center-of-mass displacement of the nucleus. The remaining term in Eq. (64) is handled in a way similar to that of the B_2 terms.

The expression for the total energy $\langle \Psi | \bar{H} | \Psi \rangle$ is now almost of the form (66). The term involving E is

$$\int d\alpha' (\alpha | \bar{H} | \alpha') = N(\alpha)(\{H\} - E),$$

while in the desired form the energy stands alone. If $N(\alpha) = \int d\alpha' (\alpha | \alpha')$ varies slowly with α so that its derivatives may be neglected, then variation with respect to f^* and division by $N(\alpha)$ yields the second-order differential equation for f,

$$\left[\{\bar{H}\} - \frac{1}{2}\left(\frac{d}{d\alpha}\{\bar{H}\}_1\right) + \frac{1}{4}\left(\frac{d^2}{d\alpha^2}\{\bar{H}\}_2\right)\right] f + \frac{d}{d\alpha}\left[\tfrac{1}{2}\{\bar{H}\}_2 + \frac{\{\bar{Q}\bar{H}\}_1^2}{\{\bar{Q}\bar{H}\bar{Q}\} \mp \{\bar{Q}^2\bar{H}\}}\right]\frac{d}{d\alpha} f(\alpha) = 0. \tag{74}$$

The two choices of sign correspond to the two possibilities of Eqs. (70). Anticipating the arguments of Sec. II D below that the derivatives of $\{H\}_i$ are small, we write Eq. (74) as

$$(\{H\} - E) f - \frac{1}{2}\frac{d}{d\alpha}\left[-\{\bar{H}\}_2 - \frac{2\{\bar{Q}\bar{H}\}_1^2}{\{\bar{Q}\bar{H}\bar{Q}\} \mp \{\bar{Q}^2\bar{H}\}}\right]\frac{d}{d\alpha} f(\alpha) = 0. \tag{75}$$

The mass parameters are identified immediately,

$$\frac{1}{B} = -\{\bar{H}\}_2 - \frac{2\{\bar{Q}\bar{H}\}_1^2}{\{\bar{Q}\bar{H}\bar{Q}\} \mp \{\bar{Q}^2\bar{H}\}}. \tag{76a}$$

The upper sign refers to the region $E > V(\alpha)$, and the lower sign to $E < V(\alpha)$.

The potential energy of deformation has the form

$$V(\alpha) = \{H\} = \frac{\int d\alpha' (\alpha | H | \alpha')}{\int d\alpha' (\alpha | \alpha')}. \tag{76b}$$

For some comments on the potential energy function see Secs. III and V below.

D. Small Quantities

The derivation of the expressions for β, Eqs. (59) and (60), and the reduction of the total energy (64) to the desired Hermitian form necessitated assumptions about the dependence of the spatial matrix elements on α and α'. In particular the assumption was made that for fixed α these matrix elements were sharply peaked about $\alpha' = \alpha$. This enabled us to expand $f(\alpha')$ and $\beta(\alpha')$ about the point $\alpha' = \alpha$ and to retain only the leading terms in these expansions.

A preliminary numerical study[18] of the overlap function $(\alpha | \alpha')$ using harmonic-oscillator wave functions supports the assumption that the dependence on $(\alpha' - \alpha)$ is very strong and that the falloff with $(\alpha' - \alpha)$ becomes more rapid as A increases.

In connection with these assumptions it is useful to discuss next the expansion parameters of the theory. Consider the various matrix elements $(\alpha | \mathcal{O} | \alpha')$ and, in particular, the normalization matrix element $(\alpha | \alpha')$. Expanded in a Taylor series in $(\alpha' - \alpha)$ this is

$$(\alpha | \alpha') = 1 + (\alpha' - \alpha)\langle \partial \rangle + \frac{(\alpha' - \alpha)^2}{2!}\langle \partial^2 \rangle + \cdots, \tag{77}$$

where

$$\partial \equiv \frac{\partial}{\partial \alpha}$$

and

$$\langle \mathcal{O} \rangle \equiv (\alpha | \mathcal{O} | \alpha) . \tag{78}$$

Furthermore

$$\langle \partial \rangle = \frac{1}{2} \frac{\partial}{\partial \alpha} \langle 1 \rangle = 0 . \tag{79}$$

For a sufficiently collective system the overlap $(\alpha | \alpha')$ is expected to be a rapidly decreasing function of $|\alpha - \alpha'|$.

With a Gaussian falloff, discussed for example by Griffin and Wheeler,[2] Brink and Weiguny,[8] Klein,[6] and by Wong,[9] to express this feature, Eq. (77) may be written

$$(\alpha | \alpha') \approx e^{-(\alpha' - \alpha)^2 / \Delta^2} \tag{80}$$

with

$$\Delta^2(\alpha) = -2/\langle \partial^2 \rangle . \tag{81}$$

The quantity Δ is expected to be small for large-A collective systems. It depends weakly[18] upon α and is taken to be constant. Similar results have been found for rotations by Sharon.[19]

If $\mathcal{O}$ is a few-body operator, then the falloff with $|\alpha' - \alpha|$ is dominated by the "core" and the same characteristic falloff "distance" Δ should obtain. This suggests the expansion

$$(\alpha | \mathcal{O} | \alpha') = e^{-(\alpha' - \alpha)^2 / \Delta^2} \times \left[\mathcal{O}_0 + (\alpha' - \alpha) \mathcal{O}_1 + \frac{(\alpha' - \alpha)^2}{2!} \mathcal{O}_2 + \cdots \right] . \tag{82}$$

Comparison with the Taylor series

$$(\alpha | \mathcal{O} | \alpha') = \langle \mathcal{O} \rangle + (\alpha' - \alpha) \langle \mathcal{O} \partial \rangle + \frac{(\alpha' - \alpha)^2}{2!} \langle \mathcal{O} \partial^2 \rangle + \cdots \tag{83}$$

yields

$$\mathcal{O}_0 = \langle \mathcal{O} \rangle , \tag{84a}$$

$$\mathcal{O}_1 = \langle \mathcal{O} \partial \rangle , \tag{84b}$$

$$\mathcal{O}_2 = \langle \mathcal{O} \partial^2 \rangle - \langle \mathcal{O} \rangle \langle \partial^2 \rangle , \tag{84c}$$

and

$$\mathcal{O}_3 = \langle \mathcal{O} \partial^3 \rangle - 3 \langle \mathcal{O} \partial \rangle \langle \partial^2 \rangle . \tag{84d}$$

The curly bracket notation (61) may be approximately expressed in terms of the $\mathcal{O}_i$ as follows:

$$\{\mathcal{O}\} \equiv \{\mathcal{O}\}_0 = \langle \mathcal{O} \rangle - \frac{1}{2} \frac{1}{\langle \partial^2 \rangle} [\langle \mathcal{O} \partial^2 \rangle - \langle \mathcal{O} \rangle \langle \partial^2 \rangle] , \tag{84e}$$

$$\{\mathcal{O}\}_1 = \frac{\langle \mathcal{O} \partial \rangle}{\langle \partial^2 \rangle} + \frac{1}{2 \langle \partial^2 \rangle^2} [\langle \mathcal{O} \partial^3 \rangle - 3 \langle \mathcal{O} \partial \rangle \langle \partial^2 \rangle] , \tag{84f}$$

and

$$\{\mathcal{O}\}_2 = -\frac{\langle \mathcal{O} \rangle}{\langle \partial^2 \rangle} + \frac{3}{2} \frac{1}{\langle \partial^2 \rangle^2} [\langle \mathcal{O} \partial^2 \rangle - \langle \mathcal{O} \rangle \langle \partial^2 \rangle] . \tag{84g}$$

The basic assumption is that the expansion coefficients $\mathcal{O}_i$ in Eqs. (84a)–(84d) do not increase rapidly as the index i increases. Then, for small Δ (collectivity assumption), the series (82) may be truncated after a few terms. Some guidance on the number of terms to be retained can be obtained by studying translational motion, where the correct mass parameter is known. This special case is discussed at length in Sec. III below. Pending that discussion, we generally keep terms through those of the "fluctuation" form, as in Eqs. (84e)–(84g).

Another useful "distance" in the theory is the wavelength associated with the collective wave function f. This is the length (i.e., range of deformations) over which there is a significant change in f, such that $|\Delta f / f| \approx 1$ or $|f'| \approx |f/L|$. For a suitably collective nucleus, $L \gg \Delta$. In expanding $f(\alpha')$ about $\alpha' = \alpha$, as done above for example in the total energy expression (64), the expansion parameter is Δ / L. In the energy we have kept such terms through order Δ^2 / L^2. This yields a second-order differential equation for f.

A third "distance" of interest is associated with the variation of the diagonal matrix element $(\alpha | \mathcal{O} | \alpha) \equiv \langle \mathcal{O} \rangle$ with α. Such a variation will be milder than that associated with the related form $(\alpha | \mathcal{O} | \alpha')$, which is characterized by the falloff distance Δ. If $(\alpha | \mathcal{O} | \alpha)$ varies appreciably only over the range D, then we expect Δ / D to be a small number. This ratio will be useful in evaluating outside derivatives of matrix elements, such as appear in the differential equation for f, Eq. (74). Note that for the case of translations D is infinite (Sec. III). D is also infinite for vibrations for the special case $\mathcal{O} = 1$.

Equation (74) reduces to the simple Peierls-Yoccoz[3] form for $\beta = 0$ ($A = B_1 = B_2 = 0$) if $D \gg \Delta$. If $\beta = 0$, Eq. (74) is

$$\left[\{\overline{H}\} - \frac{1}{2} \left(\frac{d}{d\alpha} \{\overline{H}\}_1 \right) + \frac{1}{4} \left(\frac{d^2}{d\alpha^2} \{\overline{H}\}_2 \right) + \frac{d}{d\alpha} \left(\tfrac{1}{2} \{\overline{H}\}_2 \right) \frac{d}{d\alpha} \right] f = 0 . \tag{85}$$

Equations (84e) and (84f) for $\{\overline{H}\}_1$ and $\{\overline{H}\}_2$ may be written in terms of Δ as

$$\{\overline{H}\}_1 = \tfrac{1}{2} \Delta^2 \langle \overline{H} \partial \rangle + \tfrac{1}{8} \Delta^4 (\langle \overline{H} \partial^3 \rangle - 3 \langle \overline{H} \partial \rangle \langle \partial^2 \rangle) \tag{86a}$$

and

$$\{\overline{H}\}_2 = \tfrac{1}{2} \Delta^2 \langle \overline{H} \rangle + \tfrac{3}{8} \Delta^4 (\langle \overline{H} \partial^2 \rangle - \langle \overline{H} \rangle \langle \partial^2 \rangle) . \tag{86b}$$

If the overlap falloff parameter Δ does not depend too strongly on the deformation, then derivatives of $\{\overline{H}\}_1$ and $\{\overline{H}\}_2$ with respect to α carry factors of Δ/D. These terms will then be small compared with $\{\overline{H}\}$, so that Eq. (85) becomes

$$\{\overline{H}\}f+\frac{d}{d\alpha}\frac{1}{2}\{\overline{H}\}_2\frac{d}{d\alpha}f=0 \tag{87}$$

as the equation for f with $\beta=0$. The mass parameter in this case is

$$\frac{1}{B}=-\{\overline{H}\}_2 \tag{88}$$

or since

$$\{\overline{H}\}_2=\tfrac{1}{2}\Delta^2\langle\overline{H}\rangle+\tfrac{3}{8}\Delta^4(\langle H\partial^2\rangle-\langle H\rangle\langle\partial^2\rangle), \tag{89}$$

we find

$$\frac{1}{B}=+\frac{\langle\overline{H}\rangle}{\langle\partial^2\rangle}-\frac{3}{2}\frac{\langle H\partial^2\rangle-\langle H\rangle\langle\partial^2\rangle}{\langle\partial^2\rangle^2}. \tag{90}$$

For the case of a sufficiently large mass parameter B (static approximation), the differential equation (87) provides the result

$$\{\overline{H}\}\approx 0 \tag{91}$$

or

$$E\approx H-\frac{1}{2}\frac{\langle H\partial^2\rangle-\langle H\rangle\langle\partial^2\rangle}{\langle\partial^2\rangle}. \tag{92}$$

This equation neglects the kinetic contribution to E. Note that in Eq. (90) the energy E appears only in the expectation value $\langle\overline{H}\rangle$ and not in the second term. Substitution of Eq. (92) for E into Eq. (90) finally yields

$$B_{\mathrm{PY}}=-\frac{\langle\partial^2\rangle^2}{\langle H\partial^2\rangle-\langle H\rangle\langle\partial^2\rangle}, \tag{93}$$

which is the analog of the Peierls-Yoccoz moment of inertia formula, Eq. (16).

An alternative method of evaluating Eq. (76) is to compute the integrals such as $\{\overline{H}\}_2=\int d\alpha'(\alpha'-\alpha)^2\times(\alpha|\overline{H}|\alpha')$ directly. Such a program, which avoids any doubts about convergence of the expansions discussed above, is currently being investigated.[18]

III. APPLICATION TO TRANSLATIONAL MOTION

In this case the collective motion of interest is the uniform translation of the nucleus as a whole. There is no Lagrange multiplier equivalent to that given in Eq. (37) for the vibrational case. Rather, from a wave function belonging to the system Hamiltonian H another determinant localized at a different point is obtained by the transformation

$$\psi(\vec{\mathbf{r}}_1\cdots\vec{\mathbf{r}}_A)\to\hat{\psi}(\vec{\mathbf{r}}_{\mathrm{int}};R-Z)$$
$$=\hat{\psi}(\vec{\mathbf{r}}_1-Z\hat{z},\ldots,\vec{\mathbf{r}}_A-Z\hat{z}). \tag{94}$$

Here Z is a collective coordinate (analogous to α) representing the displacement in the z direction of the z component of the center-of-mass

$$R\equiv\frac{1}{A}\sum_{i=1}^{A}z_i, \tag{95}$$

and $\vec{\mathbf{r}}_{\mathrm{int}}$ represents internal nuclear coordinates. In Eqs. (94) and (95) we have restricted ourselves for simplicity of notation to displacements in the z direction as indicated.

The intrinsic wave function is provided with a small mean center-of-mass motion[16] $\langle P\rangle$, where P is the center-of-mass momentum operator in the z direction. The generator Hamiltonian becomes in this case

$$H+\tilde{\alpha}Q-\beta\dot{Q}\to H-vP, \tag{96}$$

where v is a Lagrange multiplier. If the Hartree-Fock approximation is employed, the determinantal solution for small v is

$$\tilde{\psi}(\vec{\mathbf{r}}_{\mathrm{int}};R-Z;v)=e^{i\Lambda}\hat{\psi}(\vec{\mathbf{r}}_{\mathrm{int}};R-Z), \tag{97}$$

where the single-particle operator Λ satisfies

$$i(\mathrm{ph}|[H,\Lambda]|0)=v(\mathrm{ph}|P|0). \tag{98}$$

Equation (98) is analogous to Eq. (40). Using the expression for P as a commutator of H and R,

$$P=iM[H,R], \tag{99}$$

where M is the nuclear mass, we find

$$\Lambda=Mv[R-g(Z)]\equiv Mv\overline{R}, \tag{100}$$

where g is not a particle operator. If β is identified with Mv, the intrinsic wave function becomes

$$\tilde{\psi}(\vec{\mathbf{r}}_{\mathrm{int}};R-Z;\beta)=e^{i\beta\overline{R}}\hat{\psi}(\vec{\mathbf{r}}_{\mathrm{int}};R-Z), \tag{101}$$

and the trial wave function is

$$\Psi(\vec{\mathbf{r}})=\int dZ f(Z)e^{i\beta\overline{R}}\hat{\psi}(\vec{\mathbf{r}}_{\mathrm{int}};R-Z). \tag{102}$$

The function g is to be determined in accordance with the discussion of Sec. II. Minimizing the total energy simultaneously with respect to f and β, the formulas of Sec. II are recovered, with $\overline{Q}$ replaced by $\overline{R}$. The function g should then be chosen [see Eq. (44)] such that

$$\{[R-g(Z)]\overline{H}\}=0. \tag{103}$$

If

$$g(Z)=Z \tag{104}$$

then Eq. (103) is satisfied. This can be seen by

expanding the curly bracket notation

$$\{(R-Z)\bar{H}\} \equiv \frac{\int dZ' \int d\vec{r}_{\rm int} dR\,(R-Z)\hat{\psi}^*(\vec{r}_{\rm int};R-Z)\bar{H}\hat{\psi}(\vec{r}_{\rm int};R-Z')}{\int dZ' \int d\vec{r}_{\rm int} dR\,\hat{\psi}^*(\vec{r}_{\rm int};R-Z)\hat{\psi}(\vec{r}_{\rm int};R-Z')} \tag{105}$$

and noting that the $d\vec{r}_{\rm int}dR$ integrals are functions of $(Z-Z')$ only. (Note H is the true Hamiltonian and hence translationally invariant.) The result of the Z' integration in Eq. (105) is therefore independent of Z, and we may take $Z=0$. Then

$$\{(R-Z)\bar{H}\} = \{R\bar{H}\}_{Z=0}\,, \tag{106}$$

with the understanding that on the right-hand side of Eq. (106) Z is to be set equal to zero in the wave function

$$\{R\bar{H}\}_{Z=0} = \frac{\int dZ' \int d\vec{r}_{\rm int} dR\, R\hat{\psi}^*(\vec{r}_{\rm int};R)\bar{H}\hat{\psi}(\vec{r}_{\rm int};R-Z')}{\int dZ' \int d\vec{r}_{\rm int} dR\,\hat{\psi}^*(\vec{r}_{\rm int};R)\hat{\psi}(\vec{r}_{\rm int};R-Z')}\,. \tag{107}$$

Generally, in what follows, the subscript instruction is dropped and Z is assumed to be set to zero. From parity considerations which become evident upon the expansion of Eq. (107) according to Eq. (82),

$$\{R\bar{H}\} = 0\,, \tag{108}$$

so that Eq. (103) is satisfied with the choice (104). In a similar fashion

$$\{\bar{H}\bar{Q}\} \to \{\bar{H}(R-Z')\}_{Z=0} \equiv \{\bar{H}\bar{R}\}\,, \tag{109a}$$

$$\{\bar{Q}\bar{H}\bar{Q}\} \to \{R\bar{H}(R-Z')\}_{Z=0} \equiv \{R\bar{H}\bar{R}\}\,, \tag{109b}$$

$$\{\bar{Q}^2\bar{H}\} \to \{R^2\bar{H}\}_{Z=0} \equiv \{R^2\bar{H}\}\,, \tag{109c}$$

$$\{\bar{Q}\bar{H}\}_1 \to \{R\bar{H}Z'\}_{Z=0} \equiv \{R\bar{H}\}_1\,, \tag{109d}$$

where Z' is an integration variable. The expressions (109) will be used below. Using Eqs. (104) and (100) the trial wave function may finally be written

$$\Psi(\vec{r}) = \int dZ\, f(Z) e^{i\beta(R-Z)}\hat{\psi}(\vec{r}_{\rm int};R-Z)\,. \tag{110}$$

Let us anticipate the final result. Since the correct total energy is

$$E = E_0 + \frac{k^2}{2M}\,, \tag{111}$$

where E_0 is independent of k, and M is the nuclear mass, the choices

$$f(Z) = e^{ikZ} \tag{112}$$

and

$$\beta(Z) = k \tag{113}$$

must be correct. In this case

$$\Psi \equiv \Psi_k(\vec{r}) = e^{ikR}\int dZ\,\hat{\psi}(\vec{r}_{\rm int};R-Z)$$

$$= e^{ikR}\int dZ\,\hat{\psi}(\vec{r}_{\rm int};Z) \tag{114}$$

so that

$$\frac{(\Psi_k|H|\Psi_k)}{(\Psi_k|\Psi_k)} = \frac{(\Psi_k|H_{\rm int}+P^2/2M|\Psi_k)}{(\Psi_k|\Psi_k)}$$

$$= E_0 + \frac{k^2}{2M}\,, \tag{115}$$

where $H_{\rm int}$ operates only on the internal coordinates and P is the total momentum operator.

It is now necessary to show that the expressions (112) and (113) for f and β follow from the formalism discussed in Sec. II, and that consequently the mass-parameter formula (76) in fact gives the correct result $B=M$.

Consider the total energy Eq. (47) specialized to translations. The integration $d\vec{r}$ gives a function of $(Z-Z')$ only, so that a variation with respect to f^* yields

$$\int dZ' f(Z')h(Z'-Z) - \lambda\int dZ' f(Z')n(Z'-Z) = 0\,, \tag{116}$$

where

$$h(Z'-Z) = \int d\vec{r}_{\rm int} dR\,\tilde{\psi}(\vec{r}_{\rm int};R-Z)H\tilde{\psi}(\vec{r}_{\rm int};R-Z')\,, \tag{117}$$

$$n(Z'-Z) = \int d\vec{r}_{\rm int} dR\,\tilde{\psi}(\vec{r}_{\rm int};R-Z)\tilde{\psi}(\vec{r}_{\rm int};R-Z')\,, \tag{118}$$

and λ is a Lagrange multiplier for the normalization. A solution may be obtained with the exponential form,[20]

$$f(Z') = C\,e^{ikZ'}\,, \tag{119}$$

where C is a constant. Rewriting Eq. (119) as

$$f(Z') = C\,e^{ikZ}\,e^{ik(Z'-Z)} \tag{120}$$

and substituting in Eq. (116) gives

$$\lambda=\lambda_k=\frac{\int dZ\, e^{ikZ}h(Z)}{\int dZ\, e^{ikZ}n(Z)}. \tag{121}$$

Each of the two integrals on the right-hand side of Eq. (121) is just a number, so that with the choice $\lambda=\lambda_k$, $f=Ce^{ikZ}$ is a solution of Eq. (116). Writing Eq. (121) in detail gives

$$\lambda_k=E_k, \tag{122}$$

the total energy.

To see that the general result for β given by Eq. (63) agrees with Eq. (116) we make use of Eqs. (108) and (109), so that

$$\beta=i\frac{[ik\{R^2\bar{H}\}\{R\bar{H}\}_1+ik\{R\bar{H}(R-Z)\}\{R\bar{H}\}_1]}{\{R\bar{H}(R-Z)\}^2-\{R^2\bar{H}\}^2}. \tag{123}$$

Further simplified, Eq. (123) becomes

$$\beta=-k\frac{\{R\bar{H}\}_1}{\{R\bar{H}R\}-\{R^2\bar{H}\}-\{R\bar{H}\}_1}. \tag{124}$$

Evidently $\beta=k$ if $\{R\bar{H}R\}-\{R^2\bar{H}\}$ vanishes. Using Eq. (99) to express the commutator of H and R in terms of P, we have

$$\{R\bar{H}R-R^2\bar{H}\}=-\frac{i}{M}\{RP\}=-\frac{i}{M}\frac{\int dZ\,(0|RP|Z)}{N(0)}$$
$$=\frac{1}{M}\frac{\int dZ\,(0|R\,\partial/\partial Z|Z)}{N(0)}=0. \tag{125}$$

Therefore the formal result for β (63) is correct in the translational case. In obtaining the result (125), use has been made of the fact that

$$P\equiv -i\frac{\partial}{\partial R}=i\frac{\partial}{\partial Z}. \tag{126}$$

The last step follows, since P operates on a function of $R-Z$ only.

Similarly the total energy expression

$$E_k=\frac{\langle\Psi_k|H|\Psi_k\rangle}{\langle\Psi_k|\Psi_k\rangle}$$

[see Eq. (52)] gives the result (111). Using $\beta=k$,

$$E_k=\frac{\int dZ\, e^{ikZ}\left((0|H|Z)-\frac{1}{2}ik[(0|RH|Z)-(0|H(R-Z)|Z)]\right)}{\int dZ\, e^{ikZ}\left((0|Z)-\frac{1}{2}ik[(0|R|Z)-(0|(R-Z)|Z)]\right)}. \tag{127}$$

Keeping terms through k^2 and using

$$\int dZ\,(0|H|Z)Z=0, \tag{128}$$

$$\int dZ\left(0\left|\frac{\partial}{\partial R}\right|Z\right)=0, \tag{129}$$

and

$$\int dZ\,(0|P|Z)Z=-i\int dZ\,(0|Z), \tag{130}$$

we have as expected

$$E_k=\frac{\int dZ\,(0|H|Z)}{\int dZ\,(0|Z)}+\frac{k^2}{2M}=\{H\}+\frac{k^2}{2M}. \tag{131}$$

It is interesting to note that the total energy at rest, Eq. (131) with $k=0$, which can be expressed as

$$E_0=\frac{\int dZ(0|H_{\rm int}|Z)}{\int dZ(0|Z)}+\frac{1}{2M}\frac{\int dZ\,(0|P^2|Z)}{\int dZ\,(0|Z)} \tag{132}$$

reduces to

$$E_0=\frac{\int dZ\,(0|H_{\rm int}|Z)}{\int dZ\,(0|Z)}=\{H_{\rm int}\}, \tag{133}$$

since

$$\int dZ\,(0|P^2|Z)=\lim_{z_0\to\infty}\left(0\left|\frac{\partial}{\partial Z}\right|Z\right)\Big|_{-z_0}^{z_0}=0. \tag{134}$$

Expanding (133) through use of Eqs. (84) we have

$$E_0=\langle H_{\rm int}\rangle-\frac{1}{2}\frac{1}{\langle P^2\rangle}(\langle H_{\rm int}P^2\rangle-\langle H_{\rm int}\rangle\langle P^2\rangle)+\cdots. \tag{135}$$

To obtain a simple comparison with the expectation value of H,

$$\langle H\rangle=\langle H_{\rm int}\rangle+\frac{\langle P^2\rangle}{2M}, \tag{136}$$

assume that the wave functions with respect to which the expectation values in Eqs. (135) and (136) are calculated separate into a produce of a center-of-mass and an intrinsic part.

Then

$$E_0\approx\langle H_{\rm int}\rangle. \tag{137}$$

This formula is in fact exact for such a separable wave function. Thus the general formulation (131) for the total energy is an improvement over the expectation value of H, in that it compensates for extra energy of center-of-mass localization which is present in Eq. (136).

The kinetic term of Eq. (132) vanishes identically. However, for other modes of collective motion it will not be possible to evaluate such terms exactly. This makes it interesting to see if the energy in the translational case is improved when Eq. (132) is evaluated in an approximate way. The integral $\int dZ(0|P^2|Z)$ may be expanded by using Eqs. (84). Then, continuing to use separable wave functions

$$E_0 = \langle H\rangle - \frac{1}{4M}\frac{1}{\langle P^2\rangle}(\langle P^4\rangle - \langle P^2\rangle^2). \tag{138}$$

The expression $\langle P^4\rangle - \langle P^2\rangle^2$ is non-negative (Schwartz's inequality) so even in this approximate calculation E_0 is an improvement over $\langle H\rangle$. This leads us to anticipate that in the case of vibrational motion the potential energy will be given by the expectation value $\langle H\rangle$ minus a positive quantity. We return below to a discussion of approximate results in the translational problem, but first we verify that the formalism of Sec. II does predict the correct translational result.

Substitution of the appropriate quantities into Eq. (76) yields the equation for the mass parameter

$$\frac{1}{B} = -\{\bar{H}\}_2 - \frac{2\{R\bar{H}\}_1^2}{\{R\bar{H}(R-Z)\} - \{R^2\bar{H}\}}. \tag{139}$$

The term $\{R\bar{H}\}_1$ may be manipulated in the following way:

$$\{R\bar{H}\}_1 = \int dZ \int d\vec{r}_{\rm int} dR\, Z\hat{\psi}^*(R)R\bar{H}\hat{\psi}(R-Z). \tag{140}$$

Changing variables and using

$$(Z|(R-Z)\bar{H}|0) = (0|\bar{H}(R-Z)|Z) \tag{141}$$

we have

$$\{R\bar{H}\}_1 = -\{\bar{H}R\}_1 + \{\bar{H}\}_2. \tag{142}$$

The commutation relation between H and R allows this expression to be written as

$$\{R\bar{H}\}_1 = \frac{i}{2M}\{P\}_1 + \tfrac{1}{2}\{\bar{H}\}_2. \tag{143}$$

The bracket containing the momentum operator is reduced by an integration by parts,

$$\{P\}_1 = i\frac{\int dZ\, Z(0|\partial/\partial Z|Z)}{dZ\,(0|Z)} = -i, \tag{144}$$

so that substitution of Eq. (143) into the mass formula (139), with the result (125), yields

$$\frac{1}{B} = \frac{1}{M}, \tag{145}$$

the correct mass.

The step leading to the left-hand side of Eq. (141) depends upon the translational invariance of H, as does the fact that such quantities as $\{R\bar{H}\}_1$, are independent of Z. The result (145) is therefore obtained when the true H is used, but generally not if a shell-model Hamiltonian is substituted in its place.

The first term in Eq. (139) is equivalent to the Peierls-Yoccoz result ($\beta = 0$) for the case of translations [see Eqs. (88) and (93)]. In terms of P, the Peierls-Yoccoz mass parameter is, using Eqs. (126) and (93),

$$M_{\rm PY} = \frac{\langle P^2\rangle^2}{\langle HP^2\rangle - \langle H\rangle\langle P^2\rangle}. \tag{146}$$

To obtain the exact translational result (145) it was necessary (1) to argue that the combination of terms $\{R\bar{H}R\} - \{R^2\bar{H}\}$ occurring in the denominator of Eq. (139) vanished exactly and (2) to manipulate the integral $\{R\bar{H}\}_1$. We can anticipate, however, that for the case of vibration (Sec. IV) where the symmetry properties belonging to translation are generally lacking, the terms $\{\bar{Q}\bar{H}\bar{Q}\} - \{\bar{Q}^2\bar{H}\}$ and $\{\bar{Q}\bar{H}\}$ must be treated approximately. It will therefore be useful to study the translational case, where the mass is known, in an approximate manner. This will provide a test of particular truncations of the expansion of the overlap matrix elements as in Eq. (82).

Using the first equality in Eq. (125) to reduce the combination of terms $\{\bar{R}\bar{H}\bar{R} - \bar{R}^2\bar{H}\}$, the curly brackets of Eq. (139) may be expanded in accordance with Eqs. (84) as:

$$\{RP\} \approx \langle RP\rangle - \frac{1}{2}\frac{\langle RP^3\rangle - \langle RP\rangle\langle P^2\rangle}{\langle P^2\rangle}, \tag{147a}$$

$$\{R\bar{H}\}_1 \approx -i\frac{\langle R\bar{H}P\rangle}{\langle P^2\rangle} + \frac{i}{2}\frac{\langle R\bar{H}P^3\rangle - 3\langle R\bar{H}P\rangle\langle P^2\rangle}{\langle P^2\rangle^2}, \tag{147b}$$

$$\{\bar{H}\}_2 \approx \frac{\langle\bar{H}\rangle}{\langle P^2\rangle} - \frac{3}{2}\frac{\langle HP^2\rangle - \langle H\rangle\langle P^2\rangle}{\langle P^2\rangle^2}. \tag{147c}$$

To the order given in Eq. (147a)

$$\{R\bar{H}R - R^2\bar{H}\} = -\frac{i}{M}\{RP\} = 0, \tag{148}$$

where the relations

$$\langle RP\rangle = \tfrac{1}{2}i \tag{149}$$

and

$$\langle RP^3\rangle = \tfrac{3}{2}i\langle P^2\rangle \tag{150}$$

have been used. The result (150) was shown to be exactly satisfied in Eq. (125). Under this approximation the mass equation reduced to

$$\frac{1}{B} = -\{\bar{H}\}_2 + 2\{R\bar{H}\}_1. \tag{151}$$

To evaluate the two terms in Eq. (151) nuclear wave functions must be explicitly introduced. The matrix elements in Eqs. (147b) and (147c) may be evaluated simply using a harmonic-oscillator model. In this case the wave function separates into a product of internal and center-of-mass parts[21]

$$\psi(\vec{\mathbf{r}}) = \left(\frac{M\omega}{\pi}\right)^{1/4} \psi_{\text{int}}(\vec{\mathbf{r}}_{\text{int}}) e^{-\frac{1}{2}M\omega R^2}, \tag{152}$$

where ψ_{int} is a function of relative coordinates only, M is the nuclear mass, and ω is the frequency of the well. Equation (152) gives the following results

$$\langle \bar{H} \rangle = \tfrac{1}{4}\omega, \tag{153a}$$

$$\langle R\bar{H}P \rangle = i\tfrac{3}{8}\omega, \tag{153b}$$

$$\langle P^2 \rangle = \tfrac{1}{2}M\omega, \tag{153c}$$

$$\langle P^4 \rangle = \tfrac{3}{4}(M\omega)^2, \tag{153d}$$

$$\langle P^2\bar{H} \rangle = \tfrac{3}{8}M\omega^2, \tag{153e}$$

$$\langle R\bar{H}P^3 \rangle = i\tfrac{15}{16}M\omega^2, \tag{153f}$$

and use has been made of

$$E \approx \langle H \rangle - \frac{1}{2}\frac{\langle HP^2 \rangle - \langle H \rangle \langle P^2 \rangle}{\langle P^2 \rangle} \tag{154}$$

[see Eq. (92)]. As indicated from Eq. (133) the approximation (154) is exact for the harmonic oscillator, since

$$\langle H \rangle - \frac{1}{2}\frac{\langle HP^2 \rangle - \langle H \rangle \langle P^2 \rangle}{\langle P^2 \rangle} = \langle H_{\text{int}} \rangle = \{H_{\text{int}}\} \tag{155}$$

in that case.

With Eqs. (153) and (155) we may now write out the terms in the expression for the mass

$$\frac{1}{B} \approx -\left[\frac{\langle \bar{H} \rangle}{\langle P^2 \rangle} - \frac{3}{2M}\right] + 2\left[\left(\frac{\langle \bar{H} \rangle}{2\langle P^2 \rangle} + \frac{1}{2M}\right) - \frac{3}{4M}\right] = \frac{1}{M}, \tag{156}$$

which is the correct result. The square brackets contain the expansions of $\{\bar{H}\}_2$ and $\{R\bar{H}\}_1$, respectively. The first and second terms within each bracket correspond to the first and second terms of Eqs. (147c) and (147b), and together they also produce the correct mass. The "correction" terms in Eqs. (147b) and (147c), although cancelling each other in Eq. (156), are of the same size as the leading terms ($\langle \bar{H} \rangle / \langle P^2 \rangle = 1/2M$).

To study the convergence of the expansions (84), for which Eqs. (147) give the leading terms, the curly bracket symbols may be evaluated exactly using the harmonic-oscillator wave functions. Thus, for example,

$$\{R\bar{H}\}_1 = -\frac{1}{2M}\frac{\int dZ\, Z[-\frac{3}{4}M\omega Z + \frac{1}{8}(M\omega)^2 Z^3] e^{-M\omega Z^2/4}}{\int dZ\, e^{-M\omega Z^2/4}}. \tag{157}$$

There are two terms contributing to the integral, and they correspond to the two terms of Eq. (147b) as may be verified by explicit integration. In the harmonic-oscillator model, therefore, it is enough to keep only the first two terms in the expansion of $\{R\bar{H}\}_1$, the remaining ones being identically zero. Similarly the Eqs. (147) for $\{RP\}$ and $\{\bar{H}\}_2$ are exact for the harmonic oscillator. For more realistic wave functions the truncations of Eqs. (147) will no longer be rigorously true, but they will remain useful approximations.

Taking the translational results as a guide, it would seem to be a prudent course to retain the "fluctuation" terms, as in Eqs. (147), when discussing other classes of collective motion. This is pursued further in the following section.

IV. APPLICATION TO VIBRATIONAL MOTION

In this section the general result for the mass parameter

$$\frac{1}{B} = -\{\bar{H}\}_2 - \frac{2\{\bar{Q}\bar{H}\}_1^2}{\{\bar{Q}\bar{H}\bar{Q}\} + \{\bar{Q}^2\bar{H}\}} \tag{76}$$

will be specialized to the case where the collective motion is a change in nuclear deformation. Then Q is the quadrupole operator

$$Q = \sum_{i=1}^{A} (2z_i^2 - x_i^2 - y_i^2), \tag{158}$$

which is a sum of single-particle operators. Here (x_i, y_i, z_i) refer to the (x, y, z) coordinates of the ith particle.

From Sec. II,

$$\bar{Q} \equiv Q - g(\alpha) \tag{49}$$

and

$$g(\alpha) = \frac{\{Q\bar{H}\}}{\{\bar{H}\}}. \tag{62}$$

The function g may be approximately expressed as an expectation value as follows. From Eq. (84)

$$g \approx \frac{\langle Q\bar{H} \rangle}{\langle \bar{H} \rangle}. \tag{159}$$

At the values of $\langle Q \rangle$ corresponding to the natural extrema of $\langle H \rangle$, g can be simply expressed. This is done by generating the wave functions in Eq. (76) from $H + \tilde{\alpha}Q$ [see Eq. (37)] with $\tilde{\alpha} = 0$. For these particular equilibrium deformations H does not connect the ground state to one particle-one hole states, so that Eq. (159) becomes

$$g(\alpha) \approx \langle Q \rangle. \tag{160}$$

The intrinsic wave function is then

$$\tilde{\psi} = e^{i\beta(Q - \langle Q \rangle)} \hat{\psi}(\vec{\mathbf{r}}, \alpha). \tag{161}$$

The same result for g follows from a perturbation theory treatment of the generator Hamiltonian

$$H+\tilde{\alpha}Q-\beta\dot{Q}.$$

For small β an approximate eigenfunction is

$$\psi=|0\rangle-\beta\sum_{n\neq 0}\frac{|n\rangle\langle n|\dot{Q}|0\rangle}{E_0-E_n}, \tag{162}$$

where $|n\rangle$ refers to a member of a complete set of states, with energy E_n, which are eigenfunctions of a Hamiltonian h, itself an approximation to $H+\tilde{\alpha}Q$. Defining for the moment $\dot{Q}=i[h,Q]$, we have

$$\psi=[1+i\beta(Q-\langle Q\rangle)]|0\rangle. \tag{163}$$

For small β Eq. (163) is equivalent to Eq. (161). In Eq. (76), $\overline{Q}$ is taken to have the definition

$$\overline{Q}\equiv Q-\langle Q\rangle. \tag{164}$$

We now wish to express the mass parameter in terms of expectation values. The curly bracket symbols may be expanded in the manner discussed previously. For the region $E>V(\alpha)$, the upper sign of Eq. (76) is relevant. The denominator is

$$D_1(\alpha)=\overline{Q}\overline{H}\overline{Q}-\overline{Q}^2\overline{H}\equiv\frac{\int d\alpha'(\alpha|[(Q-\alpha)\overline{H}(Q-\alpha')-(Q-\alpha)^2\overline{H}]|\alpha')}{N(\alpha)}, \tag{165}$$

where

$$\alpha'=\int d\vec{\mathbf{r}}\,\phi^*(\vec{\mathbf{r}},\alpha')Q\phi(\vec{\mathbf{r}},\alpha'), \tag{166a}$$

$$\alpha=\int d\vec{\mathbf{r}}\,\phi^*(\vec{\mathbf{r}},\alpha)Q\phi(\vec{\mathbf{r}},\alpha)\equiv\langle Q\rangle. \tag{166b}$$

Writing

$$\alpha'=\alpha+(\alpha'-\alpha),$$

Eq. (165) becomes

$$D_1(\alpha)=-i\{\overline{Q}\dot{Q}\}-\{\overline{Q}\overline{H}\}_1 \tag{167}$$

with

$$\dot{Q}=i[H,Q]. \tag{168}$$

In the case of translations, $\{\overline{Q}\dot{Q}\}$ is equivalent to $\{RP\}$ which was shown to vanish, Eq. (125). If $\{\overline{Q}\dot{Q}\}$ were to vanish, then Eq. (76) would read

$$\frac{1}{B_1}=-\{\overline{H}\}_2+2\{\overline{Q}\overline{H}\}_1,$$

analogous to the simple translational result Eq. (151). Generally, $\{\overline{Q}\dot{Q}\}$ is nonzero, so we have

$$\frac{1}{B_1}=-\{\overline{H}\}_2+\frac{2\{\overline{Q}\overline{H}\}_1^2}{i\{\overline{Q}\dot{Q}\}+\{\overline{Q}\overline{H}\}_1},\qquad E>V(\alpha) \tag{169}$$

where the expansions (84) give

$$\{\overline{H}\}_2=-\frac{\langle\overline{H}\rangle}{\langle\partial^2\rangle}+\frac{3}{2}\frac{1}{\langle\partial^2\rangle^2}(\langle H\partial^2\rangle-\langle H\rangle\langle\partial^2\rangle), \tag{170a}$$

$$\{\overline{Q}\overline{H}\}_1=\frac{\langle\overline{Q}\overline{H}\partial\rangle}{\langle\partial^2\rangle}+\frac{1}{2\langle\partial^2\rangle^2}(\langle\overline{Q}\overline{H}\partial^3\rangle-3\langle\overline{Q}\overline{H}\partial\rangle\langle\partial^2\rangle), \tag{170b}$$

$$\{\overline{Q}\dot{Q}\}=\langle\overline{Q}\dot{Q}\rangle-\frac{1}{2}\frac{1}{\langle\partial^2\rangle}(\langle\overline{Q}\dot{Q}\partial^2\rangle-\langle\overline{Q}\dot{Q}\rangle\langle\partial^2\rangle). \tag{170c}$$

Contributions through "fluctuation" terms have been retained in accordance with the discussion of Sec. III.

If the only contributions to $\dot{Q}$ arise from the commutation of Q with the kinetic part of H in Eq. (168), then $\dot{Q}$ is the single-particle operator

$$\dot{Q}=-\frac{i}{m}\sum_{i=1}^{A}\left(4z_i\frac{\partial}{\partial z_i}-2x_i\frac{\partial}{\partial x_i}-2y_i\frac{\partial}{\partial y_i}\right), \tag{171}$$

where m is the nucleon mass. The energy E which appears in Eqs. (170a) and (170b) through the definition $\overline{H}=H-E$ may be written

$$E=\{H\}+\text{kinetic energy terms}. \tag{172}$$

Neglecting the dependence of B on the kinetic energy gives

$$E\approx\{H\}\approx\langle H\rangle-\frac{1}{2}\frac{1}{\langle\partial^2\rangle}[\langle H\partial^2\rangle-\langle H\rangle\langle\partial^2\rangle], \tag{173}$$

which may be used to eliminate explicit reference to the energy in Eq. (169).

In the regions of deformation where $E<V(\alpha)$, the lower sign of Eq. (76) is appropriate. The denominator in this case is

$$D_2(\alpha)=\{\overline{Q}\overline{H}\overline{Q}\}+\{\overline{Q}^2\overline{H}\}=2\{\overline{Q}^2\overline{H}\}-i\{\overline{Q}\dot{Q}\}-\{\overline{Q}\overline{H}\}_1, \tag{174}$$

so that the mass parameter becomes

$$\frac{1}{B_2}=-\{\overline{H}\}_2+\frac{2\{\overline{Q}\overline{H}\}_1^2}{-2\{\overline{Q}^2\overline{H}\}+i\{\overline{Q}\dot{Q}\}+\{\overline{Q}\overline{H}\}_1},\qquad E<V(\alpha). \tag{175}$$

The expansions necessary for this formula are given by Eqs. (170) and

$$\{\overline{Q}^2\overline{H}\}=\langle\overline{Q}^2\overline{H}\rangle-\frac{1}{2}\frac{1}{\langle\partial^2\rangle}[\langle\overline{Q}^2\overline{H}\partial^2\rangle-\langle\overline{Q}^2\overline{H}\rangle\langle\partial^2\rangle]. \tag{170d}$$

The most difficult expectation values to handle are $\langle QH\partial^3\rangle$ occurring in Eq. (169), and $\langle Q^2H\partial^2\rangle$ occurring in Eq. (175). The partial-derivative operator is equivalent to a sum of single-particle operators, so expectation values of six-body operators are necessary in principle. In the event of replacing the real Hamiltonian H in Eqs. (169) and

(175) by a model Hamiltonian, expectation values of operators such as $QH\partial^3$ and $Q^2H\partial^2$ become expectation values of four-body operators, if the computation is performed with eigenfunctions of the model Hamiltonian. All other expectation values are less, or comparably, difficult to evaluate.

V. COMMENT ON POTENTIAL ENERGY

As mentioned in Sec. II, the potential energy surface is not given by the expectation value $(\alpha|H|\alpha)$, but rather by the expression

$$V(\alpha)=\{H\}\equiv\frac{\int d\alpha'(\alpha|H|\alpha')}{\int d\alpha'(\alpha|\alpha')}$$

$$=(\alpha|H|\alpha)$$

$$-\frac{1}{2}\frac{(\alpha|H\partial^2|\alpha)-(\alpha|H|\alpha)(\alpha|\partial^2|\alpha)}{(\alpha|\partial^2|\alpha)}+\cdots. \tag{176}$$

For the translational case the "correction" terms were shown to remove the energy of center-of-mass localization present in $\langle H\rangle$. As the Hartree-Fock value $(\alpha|H|\alpha)$ is an upper bound to the energy, one hopes that in the case of deformational motion the additional terms in Eq. (176) will tend to lower the energy surface by removing the extra energy of localization.

VI. SUMMARY

Although the idea of applying the simple generator coordinate method to nuclear vibrations has existed for some time,[2] the variational treatment of the cranking term $\beta\dot{Q}$ and the subsequent identification of two different formulas for the associated mass parameters, applicable in two physically different regions of deformation, are new extensions of this approach. We summarize below.

Generator coordinates have been used to produce intrinsic wave functions yielding specified expectation values of Q, and also of $\dot{Q}$. The requirement that the expectation value of the latter operator be, in general, nonzero, induces a collective motion on the wave function. The Hill-Wheeler wave function is then formed by integrating the intrinsic function, multiplied by a weighting function f, over the generator coordinate α. This wave function is then a functional of f and of β, the coordinate associated with $\dot{Q}$.

The energy expression is likewise a functional of f and β. These two functions are chosen in such a way that the energy be a minimum. Varying the energy with respect to β yields an integral equation containing both f and β. Using the falloff property of the overlap matrix elements $(\alpha|\mathcal{O}|\alpha')$ associated with the collectivity of the state $|\alpha)$, β may be explicitly expressed in an approximate way in terms of f. This relation is used to eliminate β from the energy expression, which finally is varied with respect to f. An integral equation for f results.

Another application of the falloff property of $(\alpha|\mathcal{O}|\alpha')$ yields a differential equation for f. This is not of the Schrödinger form, and consequently the mass parameter may not be unambiguously identified, unless certain approximate forms for f are utilized. Generally, different forms are appropriate to the classical regions $(E>V)$ on the one hand and to the classically inaccessible regions $(E<V)$ on the other. This situation leads to two expressions for the mass parameter, one valid where $E>V$, and one where $E<V$. This is to be compared to the case of the cranking model, which always assumes that there is enough energy available to generate the motion under consideration. The energy surface maintains one simple form in both regions of deformation.

The mass parameters are given by a combination of integrals over the overlap matrix elements, in the generator coordinate space. These integrals may be approximately equated to sums of expectation values of few-body operators if the matrix elements $(\alpha|\mathcal{O}|\alpha')$ falloff quickly enough with $|\alpha-\alpha'|$. Preliminary numerical work indicates that the matrix elements in fact have this behavior. These approximations, which are necessary to produce a tractable result in the case of deformations, are studied in detail for translations, where the analogous expressions may be evaluated both exactly and approximately. It is also verified that the formalism produces the known mass correctly for this special case, and that the energy for the nucleus at rest is an improvement over $\langle H\rangle$.

Finally, the general result for deformations in terms of expectation values is written down for both the classical and tunneling regions. Those terms are dropped which are expected to be small in their own right, and which are demonstrated to be small in the translational case. The final expressions are sufficiently tractable for numerical calculation.

ACKNOWLEDGMENTS

We are pleased to acknowledge valuable discussions with Professor Sir Rudolf Peierls, Professor David Thouless, Dr. Chin Fu Tsang, and Dr. Ulrich Mosel.

*Work supported in part by the U. S. Atomic Energy Commission.

[1]D. L. Hill and J. A. Wheeler, Phys. Rev. 89, 1106 (1953).
[2]J. J. Griffin and J. A. Wheeler, Phys. Rev. 108, 311 (1957).
[3]R. E. Peierls and J. Yoccoz, Proc. Phys. Soc. (London) 70, 381 (1957).
[4]R. E. Peierls and D. J. Thouless, Nucl. Phys. 38, 154 (1962).
[5]D. R. Inglis, Phys. Rev. 96, 1059 (1954); 97, 701 (1955); see also W. A. Friedman and L. Wilets, Phys. Rev. C 2, 892 (1970), for comparison of the cranking and projection approaches for rotations.
[6]A. Klein, in *Dynamic Structure of Nuclear States*, edited by D. J. Rowe *et al.* (University of Toronto Press, Canada, 1971), p. 38.
[7]F. M. H. Villars, in *Dynamic Structure of Nuclear States* (see Ref. 6), p. 3.
[8]D. M. Brink and A. Weiguny, Nucl. Phys. A120, 59 (1968).
[9]C. W. Wong, Nucl. Phys. A147, 545 (1970).
[10]D. J. Thouless and J. G. Valatin, Nucl. Phys. 31, 211 (1962).
[11]D. J. Rowe, *Nuclear Collective Motion* (Methuen and Co., Ltd., London, 1970).
[12]F. Villars and N. Schmeing-Rogerson, Ann. Phys. (N.Y.) 63, 443 (1971).
[13]H. Rouhaninejad and J. Yoccoz, Nucl. Phys. 78, 353 (1966); J. Yoccoz, in *Many-Body Description of Nuclear Structure and Reactions, Proceedings of the International School of Physics "Enrico Fermi," Course XXXVI, 1966,* edited by C. Bloch (Academic, New York, 1966).
[14]D. M. Brink, in *Proceedings of the International Conference on Clustering Phenomena in Nuclei* (International Atomic Energy Agency, Vienna, 1969).
[15]F. Tabakin, Nucl. Phys. A182, 497 (1972).
[16]F. Villars, in *Nuclear Physics, Proceedings of the International School of Physics "Enrico Fermi," Course XXIII, 1963,* edited by V. F. Weisskopf (Academic, New York, 1963).
[17]W. H. Bassichis and L. Wilets, Phys. Rev. Letters 27, 1451 (1971).
[18]P. K. Haff and L. Wilets, to be published.
[19]Y. Y. Sharon, Ph.D. thesis, Princeton University, 1965 (unpublished).
[20]G. E. Brown, *Unified Theory of Nuclear Models and Forces* (North-Holland, Amsterdam, 1967).
[21]J. P. Elliott and T. H. R. Skyrme, Proc. Roy. Soc. (London), A232, 561 (1955).

PHYSICAL REVIEW C VOLUME 7, NUMBER 3 MARCH 1973

Sensitivity of Low-Energy Three-Body Properties to the Off-Shell Two-Body t Matrix*

J. P. Lavine,† S. K. Mukhopadhyay,‡ and G. J. Stephenson, Jr.
Department of Physics and Astronomy, and Center for Theoretical Physics, University of Maryland, College Park, Maryland 20742
(Received 27 June 1972)

Direct modifications are made to the off-shell two-body t matrices which are used as input to the Faddeev-Lovelace equations for the three-body bound state and for scattering below breakup. The t matrices are modified when either momentum argument exceeds a particular value, in a manner which will maintain off-shell unitarity when it is important. In this way, we are able to test the dependence of these three-body properties on different regions of the off-shell momenta. We find a strong sensitivity for both momenta less than 2 fm^{-1}; weak, potential-dependent sensitivity when either argument is between 2 and 5 fm^{-1}, and essentially no dependence if either argument exceeds 5 fm^{-1}.

INTRODUCTION

The ambiguity in the two-nucleon scattering amplitude off the energy shell can, in principle, be resolved by studying many-body phenomena. Several authors have studied the effects on nuclear matter and on three-body properties of making phase-shift equivalent transformations on the scattering wave functions.[1] These procedures yield modifications of the two-body t matrices over the entire range of the momentum and the energy variables. To understand the manner in which a given many-body phenomenon restricts the variation in the t matrix, it is desirable to learn which regions of momentum and energy play a dominant role in the calculation. In this paper, we address ourselves to the low-energy three-nucleon problem and study the sensitivity of the binding energy and of scattering below breakup to the two-nucleon scattering amplitude in different regions of its momentum arguments.

We consider simple models of the triton within the framework of the Faddeev-Lovelace equations[2] for separable two-nucleon scattering amplitudes. The results presented here are based on modifications of the two-body t matrices through multiplication by a function of momentum and energy chosen so that off-shell unitarity could be maintained.