Collective Motions in Nuclei by the Method of Generator Coordinates*

JAMES J. GRIFFIN,† *Princeton University, Princeton, New Jersey, and Institute for Theoretical Physics, Copenhagen, Denmark*

AND

JOHN A. WHEELER, *Palmer Physical Laboratory, Princeton University, Princeton, New Jersey*

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For an A-particle system, a trial wave function is constructed of the form

$$\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_A)=\int\varphi(\mathbf{x}_1,\cdots,\mathbf{x}_A;\alpha)f(\alpha)d\alpha.$$

The preliminary nucleonic wave function, φ, solves the problem in a "construction potential." This potential depends upon a "deformation parameter" or "generator coordinate," α. The collective wave function, $f(\alpha)$, or "generator function," is folded into φ to produce a system wave function that depends only upon the coordinates, $\mathbf{x}_i$, of the particles. In the integration, the deformation parameters dissolve away. They do not appear in the final state function; they only generate it. No collective coordinates ever come into use nor do such coordinates ever have to be defined. In typical cases when the generator function contains one or more nodes, it generates nodes in the system wave function Ψ of the kind that describe collective kinetic energy. The energy of the system is extremized with respect to choice of the generator function, $f(\alpha)$. No Hamiltonian ever appears except the A-particle Hamiltonian. All nucleons are treated on the same basis whether in or above closed shells. The appropriate variational calculation leads to an integral equation or "generator wave equation" for $f(\alpha)$. This equation is solved in two limiting cases: the quadratic approximation, and the δ-function approximation. An analysis is made of the Peierls-Yoccoz procedure to calculate the effective-mass parameter in cases where the forces acting in the system are invariant with respect to translation or rotation. There is no external machinery to drive the construction potential. The effective inertia constant does not appear likely to agree in general with that calculated for the essentially different problem of particles in such a machine-driven potential, though the latter value is presumably more nearly correct for physical applications. The trial wave function in the method of generator coordinates is designed for simplicity, not for precision. It is applied in the following paper to the dilatational and shape oscillations of O^{16}.

I. INTRODUCTION; THE METHOD OF GENERATOR COORDINATES IN OUTLINE; SUMMARY

Variational Description of Collective Motion

BOHR and Mottelson[1] and others have had success in describing collective nuclear rotations and deformations in analogy to molecular rotations and deformations (Table I). For many parts of their analysis, it is unnecessary to go go back to the many-body problem. However, when one wants to determine such a quantity as the frequency of a collective vibration starting from an assumed force between nucleons or to have an explicit expression for the wave function of the system in terms of coordinates alone, it is, of course, necessary to return to first principles. Much attention has recently been given to this problem, which presents considerable mathematical complexities. The present paper seeks to assess a *variational*—and therefore approximate—method which has been put forward previously[2] to describe collective motions.

We consider a system of A-particles with coordinates $\mathbf{x}_1$, $\mathbf{x}_2$, $\cdots\mathbf{x}_A$ with a Hamiltonian function,

$$H=(\mathbf{p}_1^2/2M)+(\mathbf{p}_2^2/2M)+\cdots(\mathbf{p}_A^2/2M)+\sum_{i<k}V(r_{ik}). \quad (1)$$

We construct the trial wave function of the variational method in the following way: we replace the actual potential felt by a particle by a fictitious potential, characterized by a shape parameter, α. We solve the wave equation for individual particles moving in this potential. Out of these individual particle wave functions, we construct by formation of a determinant or otherwise a many-particle wave function

$$\text{the } \textit{nucleonic wave function}, \ \varphi_n(\mathbf{x}_1\cdots\mathbf{x}_A;\alpha). \quad (2)$$

This wave function is completely and uniquely determined once one knows the *construction potential* as a function of α. The *trial wave function* for the many body system is now taken to be given by the following expression:

$$\Psi(\mathbf{x}_1,\cdots\mathbf{x}_n)=\int\varphi_n(\mathbf{x};\alpha)f(\alpha)d\alpha. \quad (3)$$

Here the quantity, α, may be given the name of *generator coordinate*, because it serves to generate the wave function of the system. It should be emphasized, how-

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† Present address: Los Alamos Scientific Laboratory, Los Alamos, New Mexico. Grateful acknowledgment is made of a Fulbright Fellowship held in Copenhagen, 1955–1956.

[1] A. Bohr, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **26**, No. 14 (1952); A. Bohr and B. Mottelson, Kgl. Danske Videnskab. Selskab, Mat-fys. Medd. **27**, No. 16 (1953).

[2] The earliest proposal [D. L. Hill and J. A. Wheeler, Phys. Rev. **89**, 1106 (1953)] assumed a trial function that contained the velocity potential, $u(\mathbf{x})$,

$$\int\varphi(\mathbf{x},\alpha)\exp\{-i(M/\hbar)\Sigma_j u(\mathbf{x}_j)\}f(\alpha)d\alpha.$$

The present simpler and physically more reasonable form was proposed by J. A. Wheeler, *Proceedings of the 1954 Glasgow Conference on Nuclear and Meson Physics*, edited by E. H. Bellamy and R. G. Moorhouse (Pergamon Press, London and New York, 1955), pp. 42 and 43; J. A. Wheeler, Suppl. Nuovo cimento **2**, 908 (1955) and J. J. Griffin, Phys. Rev. **99**, 648(A) (1955); and has since been developed and explored in further detail by R. Peierls and J. Yoccoz, Proc. Phys. Soc. (London) **A70**, 381 (1957) and J. Yoccoz, Proc. Phys. Soc. (London) **A70**, 388 (1957).

TABLE I. Analogy between the collective nucleus and a molecule, illustrating features that can be expected to come into evidence in *any* treatment of collective motions, whether via the product type of wave function or via the generator coordinate type of wave function that is treated in this paper.

Property	Molecule	Nucleus
Individual particle state occupied by	Electron	Nucleon
Slowly varying parameters that affect energy of individual particle states	Internuclear separations; r_{12}, r_{13}, $\cdots$etc.	Parameter α and other parameters that describe in more detail the configuration of the nuclear well
Oscillation period in an example	8×10^{-15} sec in H_2	$\sim5\times10^{-21}$ sec in U
Fundamental period of motion of most energetic particle in same example	$\sim10^{-15}$ sec	$\sim0.3\times10^{-21}$ sec
Vibrational potential energy described as function of these one or more parameters by a curve or surface	$V(r_{12},r_{13},\cdots)$ = sum of energies of individual electron states plus electrostatic interactions not otherwise taken into account	Sum of energies of individual nucleon states calculated for a deformed well plus other interactions not otherwise taken into account
Vibrational or rotational kinetic energy	Mainly localized in nuclei	Increment of kinetic energy of nucleons because well is moving and nodes of individual particle wave functions are undergoing displacement
Exchange of energy between individual particle excitation and general vibration of the system can take place at point of contact between one potential surface and an adjacent one, via a radiationless transition	Mechanism for excitation to be degraded into vibrational energy; important in polyatomic molecules, where the variation of two or more parameters ordinarily allows one to arrive at a point in configuration space where two successive potential surfaces make a cusp-like contact	Mechanism for nucleonic motion to be degraded into collective motion, and conversely for energy of collective vibration to be imparted to an individual nucleon as for example in a nucleonic evaporation process. To be distinguished from direct energy exchanges between a pair of nucleons—an independent mechanism for capture and evaporation. Both contribute to the absorption component of the complex nuclear potential

ever, that this generator coordinate is not expressed or expressible as a function of the coordinates, $\mathbf{x}_1\cdots\mathbf{x}_A$. The only quantities free in determining the trial function, Ψ, are (1) the nucleonic quantum number, n, that characterizes the nucleonic state of the many particle system in the construction potential, and (2) the *generator wave function*, $f(\alpha)$, a so far undetermined function of α. We next determine this collective wave function by the requirement that the *expectation value* of the energy of the A-particle system shall be an extremum with respect to choice of the generator wave function, $f(\alpha)$:

$$\delta E=0; \quad \text{or} \quad \delta E/\delta f(\alpha)=0. \tag{4}$$

Renunciation of Any Explicit Use of a Collective Coordinate

It would be easy to imagine a more general formulation of the method of generator coordinates, in which one took a variational function of the form

$$\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_A)=\int\varphi(\mathbf{x}_1,\cdots,\mathbf{x}_A,\alpha)\times S(\mathbf{x}_1,\cdots,\mathbf{x}_A;\alpha)f(\alpha)d\alpha. \tag{5}$$

Here the function $S(\mathbf{x};\alpha)$ is considered to be fixed once and for all and to describe an extra correlation among the particles not included in the nucleonic wave function, $\varphi(\mathbf{x};\alpha)$. Our collective wave function is a special case where the function S is set equal to 1. Another special case of this more general form of wave function is obtained by substituting for the correlation function, S, the expression

$$S(\mathbf{x};\alpha)=\delta(\alpha-\xi(\mathbf{x}_1\cdots\mathbf{x}_A)). \tag{6}$$

Here δ is the Dirac delta function. The quantity $\xi(\mathbf{x}_1\cdots\mathbf{x}_A)$ is a trial expression for the collective coordinate of the state in question. For example, in the case of translational collective motion, one would insert for ξ, the expression

$$\xi=(1/A)(\mathbf{x}_1+\mathbf{x}_2+\cdots+\mathbf{x}_A). \tag{7}$$

Owing to the presence of the delta function, it is obvious that the integration over the generator coordinate, α, can be carried out at once with the result that the combined wave function has the form

$$\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_A)=\varphi(\mathbf{x};\xi(\mathbf{x}))f(\xi(x)). \tag{8}$$

This is the type of wave function used by Bohr and Mottelson, Tolhoek, Tomonaga, and others[3] in describing the collective vibrations and other collective motions. The advantages and difficulties of this type of wave function are well known. It is simple in principle but—in the case of oscillations and rotations—difficult to write out in detail. In particular, it is difficult to find a simple explicit expression for the deformation co-

[3] H. A. Tolhoek, Physica **21**, 1 (1954); S. Tomonaga, Progr. Theoret. Phys. Japan **13**, 467 (1955); Marumori, Yukawa, and Tanaka, Progr. Theoret. Phys. Japan **13**, 442 (1955); Lipkin, de Shalit, and Talmi, Nuovo cimento **2**, 773 (1955); Marumori, Progr. Theoret. Phys. Japan **14**, 608(L) (1955).

TABLE II. Comparison and contrast of the product type and generator type of wave functions for the description of collective motion.

Quantity	Product type of wave function	Generator type of wave function
Wave function	$\Psi(\mathbf{x}_1,\cdots\mathbf{x}_A)=\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha(\mathbf{x}))f(\alpha(\mathbf{x}))$	$\Psi(\mathbf{x}_1,\cdots\mathbf{x}_A)=\int\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)f(\alpha)d\alpha$
Collective variables $\alpha_2, \alpha_3, \cdots\alpha_s$	Functions of the particle variables, $\mathbf{x}_1, \cdots\mathbf{x}_A$	Parameters which describe the shape of the construction potential but which are integrated out and never appear in the final trial wave function
Number of coordinates	$A+s$ (extra coordinates) $-s$ (constraints) $=A$	Always A
Complete Hamiltonian	$\frac{\mathbf{p}_1^2}{2m}+\cdots+\frac{\mathbf{p}_A^2}{2m}+\sum_{i<k}V(r_{ik})$	$\frac{\mathbf{p}_1^2}{2m}+\cdots+\sum V(r_{ik})$
Energy operator in reduced form for treatment of collective motion	A function of collective variables, $\alpha_2, \cdots\alpha_s$, obtained explicitly or implicitly by appropriate averaging procedures	Integral wave equation for collective motion: $\int[K(\alpha,\beta)-EI(\alpha,\beta)]f(\beta)=0$
Deformation potential	A function, $V(\alpha_2,\alpha_3,\cdots)$ of the collective variables in complete analogy to the molecular vibration potential	In general a kernel, $K(\alpha_2,\beta_2;\alpha_3,\beta_3;\cdots)$ or integral operator; in certain cases reducible via the "δ-function approximation" to the form $V(\alpha_2,\alpha_3,\cdots)$

ordinate, $\xi(\mathbf{x}_1,\cdots,\mathbf{x}_A)$ in terms of the individual particle coordinates. The method of generator coordinates described in the present article is probably less accurate than the method of the product wave function. Its primary advantage is, therefore, only the one of convenience: one never deals with any expression for a collective coordinate, ξ. One never sees anything in the nature of an explicit collective coordinate. One sees only the "generator coordinate," α, which is not a coordinate at all but a parameter which describes the shape of the "construction potential." This difference in approach between the method of the "product wave function" and the present method of "generator coordinates" (Table II) is the central topic of the present paper.

Integral Wave Equation for Generator Wave Function

The present investigation consists of four parts. In Sec. II, we spell out the method of construction of the over-all wave function in more detail and the consequences of the variational principle for the choice of function $f(\alpha)$. We show that the variational principle leads to a simple integral equation for the determination for the function $f(\alpha)$, an integral equation of the following form,

$$\int[K(\alpha,\beta)-E_vI(\alpha,\beta)]f(\beta)d(\beta)=0, \tag{9}$$

where K is the so-called *energy kernel* and the I is the *overlap kernel.*

Exact Solution in the Quadratic Approximation

This *generator wave equation* can, in general, only be solved by numerical methods. However, there are two simple classes of kernel (Table III) that simplify the equation. In the one case (Sec. III), it is a good approximation to replace the kernels by mathematical expressions of the form

$$K(\alpha,\beta)=\left\{E_g+\frac{\hbar^2}{2\mathfrak{M}}[2s-4s^2(\beta-\alpha)^2]+\tfrac{1}{2}\mathfrak{M}\Omega^2\left(\frac{\beta+\alpha}{2}\right)^2\right\}\times I(\alpha,\beta), \tag{10}$$

$$I(\alpha,\beta)=\exp[-s(\alpha-\beta)^2]. \tag{11}$$

We call this case the *quadratic approximation.* For such quadratic kernels, the eigenvalue problem can be solved exactly by a natural generalization of the familiar harmonic oscillator wave functions. The energy eigenvalues are found to be given by the simple formula

$$E_v=E_g+(v+\tfrac{1}{2})\hbar\Omega-(\mathfrak{M}\Omega^2/16s)\quad(v=0,1,2,\cdots). \tag{12}$$

The generator wave function for the ground state, $v=0$, has the form

$$f_0(\alpha)=N_0\exp[-\tfrac{1}{2}(\alpha^2/a^2)];\quad a^2=\frac{\hbar}{\mathfrak{M}\Omega}-\frac{1}{4s}. \tag{13}$$

The uniform spacing of the energy levels and the quadratic form of the ratio of kernels, K/I, leads us to identify the system in question with a harmonic oscillator. The constant $\mathfrak{M}$ may be regarded as the effective mass associated with the collective motion, and the quantity Ω is to be identified with the effective frequency of the harmonic oscillator.

Differential Equation in δ-Function Approximation

In Sec. IV, we analyze the case where the integral equation reduces to the Schrödinger differential equation. We call this case the *δ-function approximation:*

$$I(\alpha,\beta)\rightarrow\delta(\alpha-\beta), \tag{14}$$

$$K(\alpha,\beta)\rightarrow-\frac{\hbar^2}{2\mathfrak{M}}\delta''(\alpha-\beta)+V\left(\frac{\alpha+\beta}{2}\right)\delta(\alpha-\beta). \tag{15}$$

TABLE III. One-dimensional generator equation: relation of the solvable cases to the general case. The generator function, $f(\alpha)$, of the generator coordinate, α, generates the collective wave function as indicated in Eq. (3).

$\frac{K}{I}=\frac{\text{energy kernel}}{\text{overlap kernel}}$ / $I(\alpha,\beta)=\text{overlap kernel}$		$E_0+\frac{1}{2}\mathfrak{M}\Omega^2\left(\frac{\beta+\alpha}{2}\right)^2$ $+\frac{\hbar^2}{2\mathfrak{M}}[2s-4s^2(\beta-\alpha)^2]$	General function of β and α (even in $\beta-\alpha$)
Simple Gauss function $\exp[-s(\alpha-\beta)^2]$	δ-function limit (s very large) (Sec. IV)	Integral equation goes over into Schrödinger differential equation.	
		Solutions given by standard harmonic oscillator functions	Solve $\frac{d}{d\alpha}\frac{\hbar^2}{2\mathfrak{M}(\alpha)}\frac{df}{d\alpha}+[E-V(\alpha)]f(\alpha)=0.$
	General value of s	Solved in III via generalized harmonic-oscillator functions. Solutions make sense only when $s>\mathfrak{M}\Omega/4\hbar$. (See Eq. (13))	Solution demands general methods of theory of integral equations or lattice approximation leading to n algebraic equations for n unknowns. Peierls' approximation uses trial solution of type $f(\alpha)=e^{ik\alpha}$ and expands expectation value of energy in form $\langle E\rangle=\frac{\langle K\rangle}{\langle I\rangle}=\frac{K_0-\frac{1}{2}K_2k^2+\cdots}{I_0-\frac{1}{2}I_2k^2+\cdots}$. Discussion in Sec. V.
General function of β and α (even in $\beta-\alpha$)			

Issue of the Effective Inertial Parameter

In trying to describe collective motions, one has several goals: (1) to construct in a simple way a wave function, $\Psi_{nv}(\mathbf{x}_1,\cdots,\mathbf{x}_A)$ that (a) depends upon particle coordinates alone but (b) brings into evidence collective motion; (2) to separate off in a separate equation the dynamics of the collective motion. One seeks a form for this equation that will show up (a) the effective inertia associated with the collective motion and (b) the restoring force, if any. By renouncing any explicit use of a collective variable, $\xi(\mathbf{x}_1,\cdots,\mathbf{x}_A)$, the method of generator coordinates achieves these goals by a method that is direct and easy, but not at all simple to check for accuracy. This issue of accuracy, at the present stage of nuclear physics, focuses primarily on the inertial parameter (Sec. V).

The method of generator coordinates is applied in the following paper to treat the dilatational and deformational oscillations of O^{16}.

II. METHOD OF GENERATOR COORDINATES AS A VARIATIONAL METHOD

Variational Method as a Means to Bring into Evidence an Elusive Degree of Freedom; Example of Resonating Group Structure

To bring into evidence the degree of freedom associated with collective motion without actually bringing onto the scene any new coordinates and to do this by a variational type of trial wave function is a problem of a very general character, not limited to collective vibrations of the nucleus. A similar problem has been faced in quite another connection in the past: how to describe the degree of freedom associated with the approach and recession of two alpha particles.[4] It is not enough to introduce as coordinate the separation of the centers of mass of two alpha particle groups,

$$\mathbf{X}=(-\mathbf{x}_1-\mathbf{x}_2-\mathbf{x}_3-\mathbf{x}_4+\mathbf{x}_5+\mathbf{x}_6+\mathbf{x}_7+\mathbf{x}_8)/4, \quad (16)$$

because the groupings of neutrons and protons into alpha particles ordinarily changes as a consequence of the collision. To meet this difficulty, it was found useful to introduce the concept of "resonating group structure." The wave function for the system was written as a superposition of terms corresponding to *all* the possible groupings of neutrons and protons into alpha particles:

$$\begin{aligned}\Psi(\mathbf{1},\mathbf{2},\cdots\mathbf{8})&=F\left(\frac{-\mathbf{1}-\mathbf{2}-\mathbf{3}-\mathbf{4}+\mathbf{5}+\mathbf{6}+\mathbf{7}+\mathbf{8}}{4}\right)\times\Phi(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{4})\Phi(\mathbf{5},\mathbf{6},\mathbf{7},\mathbf{8})\\&+F\left(\frac{-\mathbf{1}-\mathbf{2}-\mathbf{3}-\mathbf{8}+\mathbf{5}+\mathbf{6}+\mathbf{7}+\mathbf{4}}{4}\right)\times\Phi(\mathbf{1},\mathbf{2},\mathbf{3},\mathbf{8})\Phi(\mathbf{5},\mathbf{6},\mathbf{7},\mathbf{4})\\&+\cdots. \quad (17)\end{aligned}$$

Here the functions Φ represent the wave functions of alpha particles at rest—assumed known—and the function $F(\mathbf{X})$ represents a so far undetermined function of the variable $\mathbf{X}$. Thus the total wave function, Ψ, has the character of a *trial wave function*. It is the key concept to determine the "best" trial wave function of this type—best in the sense of the variational principle—by extremizing the expectation value of the energy of the system with respect to the choice of $F(\mathbf{X})$. Of course,

[4] John A. Wheeler, Phys. Rev. **52**, 1107 (1937); for other applications of the method of resonating group structure, see F. Brown, Phys. Rev. **56**, 1107 (1939); R. Buckingham and H. Massey, Proc. Roy. Soc. (London) **A179**, 123 (1941); H. Hocker, Physik. Z. **43**, 236 (1942); H. Massey and R. Buckingham, Phys. Rev. **71**, 558 (1947); also the summary in A. Rosenfeld, *Nuclear Forces* (Interscience Publishers, Inc., New York, 1949).

one cannot calculate this expectation value,

$$\langle E\rangle=\int\Psi^*\left[\frac{\mathbf{p}_1^2}{2m}+\cdots+\frac{\mathbf{p}_8^2}{2m}+\sum_{i<k}V(r_{ik})\right]\Psi d\tau\Big/\int\Psi^*\Psi d\tau, \quad (18)$$

explicitly without knowledge of $F(\mathbf{X})$. However, one *can* perform all integrations other than those which affect the separation coordinates themselves. In this way, one expresses the energy in a form that depends *only* on the functional form of $F(\mathbf{X})$. Then the demand that the energy be an extremum,

$$\delta E=0, \quad (19)$$

leads directly to an equation for the unknown function $F(\mathbf{X})$. This equation may be termed the "wave equation for the alpha-particle scattering" in the relevant approximation. The existence of such an equation in one coordinate, $\mathbf{X}$, clearly by no means implies or assumes that the same groupings emerge from the collision which entered it. On the contrary, the asymptotic behavior of the function $F(\mathbf{X})$ at large distances gives one a means to define the scattering cross section regardless of the amount of exchange that takes place at the time of collision. The consistent following out of this line of reasoning led directly to the first introduction of the scattering matrix.[4]

Briefly stated, the variational method allows one to sort out one or two variables from a larger number of variables. The most convenient technique for this purpose depends upon the nature of the problem. In the alpha-particle case, the function to be varied depended upon a separation because that separation was easily defined. In the present case, it would be conceivable to introduce an undetermined function of a suitably defined collective coordinate, but unhandy to do so because of the complications met in defining such coordinates. This is the reason for adopting in the present problem a parameter α, related, not directly to the configuration of the particles themselves, but to the shape of the effective potential in which they move. From this concept follow naturally the features of the method described here: (1) construction potential, (2) deformation parameter or generator coordinate, (3) nucleonic wave function, $\varphi(\mathbf{x}_1,\cdots,\mathbf{x}_A;\alpha)$, (4) generator wave function, $f(\alpha)$, and (5) the trial wave function formed by folding together 3 and 4.

Construction Potential and the Preliminary Nucleonic Wave Function

The kind of construction potential to be used depends upon how much of the normal nucleonic interactions we suspend in the construction of the preliminary nucleonic wave function, $\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)$. It is simplest to think at the start of the case where all interactions are suspended and where they are replaced by a potential well, $V(x,y,z;\alpha)$ (Fig. 1). The shape of this well or its extension shape or both are described by one or more parameters, α. Let $u_k(\mathbf{x};\alpha)$ denote the single particle states in this potential well. Then we fill up the lowest A states and construct the antisymmetrized nucleonic wave function

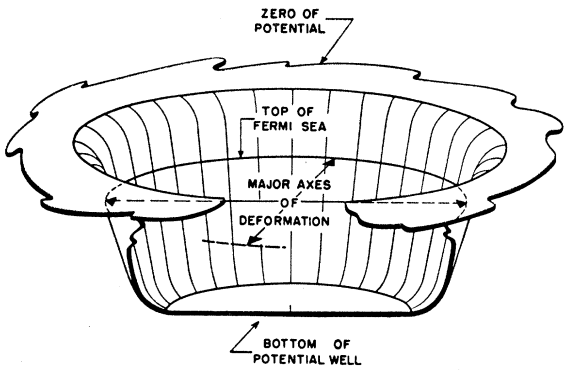

FIG. 1. Schematic representation of construction potential, $V(x,y,z;\alpha)$. The parameter α may describe a change in shape of the potential well, such as a spheroidal deformation; or a change in orientation, as in the case of a collective rotation; or a change in extension as in a dilatational vibration; or there may be several such parameters to describe simultaneously several types of collective motion.

$$\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)=(A!)^{-\frac{1}{2}}\begin{vmatrix}u_1(\mathbf{x}_1,\alpha)&\cdots&u_1(\mathbf{x}_A,\alpha)\\ \vdots&&\vdots\\ u_A(\mathbf{x}_1,\alpha)&\cdots&u_A(x_A,\alpha)\end{vmatrix}. \quad (20)$$

Much attention has been given to the calculation of such individual particle wave functions in a deformed potential well.[5]

It is interesting to compare this scheme for constructing the preliminary nucleonic wave function with the familiar procedure for building the electronic wave function for a molecule out of molecular orbitals. The intermolecular separations, $r_{ab}, r_{bc}, \cdots$, fulfill in that problem the function of the deformation coordinates, α, in this problem in one sense: they can be regarded as defining the principal features of the average field of force. In the molecular case as in the nucleonic case, one deals at this level of analysis only with an average field of force. No account is taken of the circumstance that different particles move in slightly different fields of force. But it is to be recalled that final energy values are not being calculated at this stage; one is only setting up a trial wave function which is subsequently to be used, without any thought as to where it came from, to extremize the energy of the system.

[5] Perturbation methods: James Rainwater, Phys. Rev. **79**, 432 (1950); D. L. Hill and J. A. Wheller, Phys. Rev. **89**, 1102 (1953), Figs. 14 through 23; S. Moszkowski, Phys. Rev. **99**, 803 (1955); S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **29**, No. 16 (1955); electronic machine calculations: Nilsson; K. Gottfried, thesis, Massachusetts Institute of Technology, 1955 (unpublished); Marvin Rich, Bull. Am. Phys. Soc. Ser. II, **1**, 253 (1956); electronic calculations and statistical methods, D. L. Hill and J. A. Wheeler (to be published).

Were the molecule endowed with an atmosphere of positive electrons as well as negative electrons, one would obviously use opposite effective fields of force for the two kinds of particles in the preliminary "construction potential" phase of the calculations. Similarly, in the nucleonic problem, it is reasonable to think of using different construction potentials for neutrons and protons (1) in dealing with nuclei of high charge number[6] or (2) in analyzing collective states of disturbance in which the neutrons and protons vibrate as groups relative to each other.[7] Obviously, one will count on using at least two generator coordinates in describing the collective motions of such a system.

Despite the similarities between molecular vibrations and the collective motions of the nucleus, there is one evident difference in the mathematical machinery as just outlined for the two cases. In the nuclear problem, the method of generator coordinates assigns construction potentials which every particle can follow. In the molecular case, one can define the equivalent of a construction potential for the electrons, but for the nuclei that make up the molecule, it is not convenient to define such construction potentials. There is no statistical character to the distribution of these heavy centers of mass. They are treated on quite a different footing in the analysis. In the simplest approximation, all of the kinetic energy is assigned to them.[8] In contrast, the kinetic energy of collective nuclear oscillations arises from all the particles.[9] These particles experience an increase in kinetic energy due to the changes in time of the effective potential well. This increase over and above the normal kinetic energy for a stationary configuration may be identified with the kinetic energy of the collective motion.[10]

To suspend all of the nucleonic interactions and to replace them in total by a construction potential for the definition of the preliminary nucleonic wave function, $\varphi(\mathbf{x}_1,\cdots,\mathbf{x}_A;\alpha)$, is, of course, a drastic procedure to which there are more accurate but more complicated alternatives: (1) Follow the devices of the shell model. Include the effect of the bulk of the nucleonic forces in the effective average potential, now to be our α-dependent construction potential. Recognize, however, that there remain residual interactions that couple the individual nucleon states.[11] Allow for the resultant configuration interaction in whatever detail seems reasonable in constructing the nucleonic wave function, $\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)$. Or (2), follow the formalism of Brueckner[12] in allowing for these residual nucleonic interactions and in building up an appropriate mathematical expression for the nucleonic state function—again in an α-dependent construction potential that represents the saturation part of the nucleonic interactions. We have not attempted either of these ambitious programs. Instead the following paper uses a simple Slater determinant of individual-particle wave functions to represent the nucleonic state function for the deformed potential well.

Generation of New Nodes in the System Wave Function by the Method of Generator Coordinates

When we fold the nucleonic wave function, $\varphi(\mathbf{x}_1,\cdots,\mathbf{x}_A;\alpha)$ into the generator wave function $f(\alpha)$ to give the variational wave function, $\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_A)$, we put into the final wave function as many new nodes associated with collective motion as there are nodes in

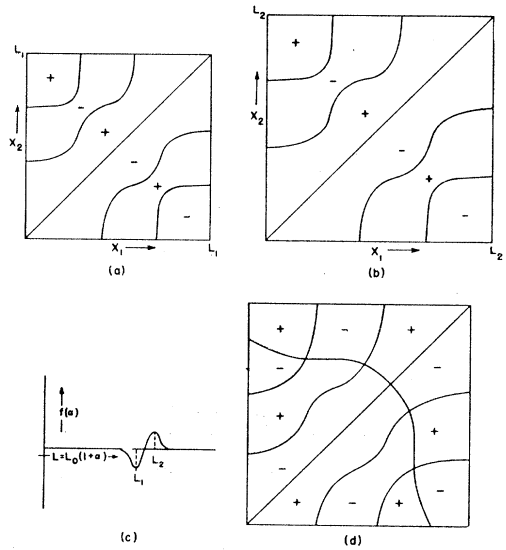

FIG. 2. Nodes in the original "nucleonic" wave function (a) and generation of a new node by folding into a generator wave function, $f(\alpha)$, which itself has one node (c). The indicated function, $f(\alpha)$, gives positive weight to the nucleonic wave function when the construction potential is dilated to the extension, $L_2=L_0(1+\alpha)$, as in diagram (b). A negative weight is attached to the contracted nucleonic wave function in (a). The superposition with opposite signs of nucleonic wave functions such as those in (a) and (b) gives a total system wave function, $\Psi(\mathbf{x}_1,\mathbf{x}_2)$, that has an extra node, as indicated in (d). The present illustration is limited to the case of two particles free to move in only one dimension. The "nucleonic wave function" in (a) and (b) is $\varphi(\mathbf{x}_1,\mathbf{x}_2;\alpha)=(2/L)\times[\sin(3\pi x_1/L)\sin(4\pi x_2/L)-\sin(4\pi x_1/L)\sin(3\pi x_2/L)]$.

[6] M. H. Johnson and E. Teller, Phys. Rev. **93**, 357(L) (1954); W. J. Swiatecki, Phys. Rev. **98**, 203 and 204 (1955).

[7] M. Goldhaber and E. Teller, Phys. Rev. **74**, 1046 (1948); J. H. D. Jensen and H. Steinwedel, Z. Naturforsch. **5a**, 413 (1950); J. S. Levinger, Rev. mex. fis. **5**, 177 (1956) and references therein cited.

[8] M. Born and J. R. Oppenheimer, Ann. Physik **84**, 457 (1927).

[9] D. R. Inglis, Phys. Rev. **96**, 1059 (1955) and **97**, 701 (1955); A. Bohr and B. R. Mottelson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **30**, No. 1 (1956); S. Moszkowski, Phys. Rev. **103**, 1328 (1956); Lipkin, de Shalit, and Talmi, Phys. Rev. **103**, 1773 (1956).

[10] D. L. Hill and J. A. Wheeler, Phys. Rev. **89**, 1102 (1953), Figs. 7 and 8.

[11] M. G. Mayer and H. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure* (John Wiley and Sons, Inc., New York, 1955); E. Feenberg, *Shell Theory of the Nucleus* (Princeton University Press, Princeton, 1955); A. M. Lane, *Handbuch der Physik* [Springer-Verlag, Berlin (to be published)].

[12] K. A. Brueckner, Phys. Rev. **100**, 36 (1955) and earlier papers therein cited; see also the analysis of Brueckner's method by H. A. Bethe, Phys. Rev. **103**, 1353 (1956).

$f(\alpha)$. Figure 2 illustrates in a very much over-simplified way the mechanism by which nodes are introduced into the wave function in the $3n$-dimensional configuration space. These nodes are ordinarily associated, not with individual-particle excitations, but with excitations of the system as a whole.

Where the new nodes appear in the newly generated wave function depends, of course, upon the choice of construction potential and deformation parameters that one has made in the first place. Natural choices present themselves for these quantities in the nuclear problem, where it is fairly clear what to do to describe dilatations, shape vibrations, and collective rotations. However, one could imagine other conceivable applications of a purported method for the analysis of collective motions where it would not be at all obvious what to use for the deformation parameters. In such problems, the method of generator coordinates provides no magic machinery that can be operated without the exercise of judgment.

Use of the Variational Principle to Determine the Generator Wave Function, $f(\alpha)$

We shall now find the trial function that extremizes the energy,

$$E=\int \Psi^*(\mathbf{x})H\Psi(\mathbf{x})d^3x_1\cdots d^3x_A \Big/ \int \Psi^*(\mathbf{x})\Psi(\mathbf{x})d^3x_1\cdots d^3x_A, \quad (21)$$

where the Hamiltonian contains particle coordinates only:

$$H=\frac{\mathbf{p}_1^2}{2m}+\cdots+\frac{\mathbf{p}_A^2}{2m}+\sum_{i<k}V(r_{ik}). \quad (22)$$

We substitute the expression for the trial wave function in terms of the nucleonic wave function—presumed to be known—and the still adjustable generator wave function, $f(\alpha)$:

$$\Psi^*(\mathbf{x})=\int \varphi^*(\mathbf{x};\alpha)f^*(\alpha)d\alpha,$$
$$\Psi(\mathbf{x})=\int \varphi(\mathbf{x};\beta)f(\beta)d\beta. \quad (23)$$

Then in expression (21) for the energy all quantities dependent upon x are known, and the integrations over these variables can be performed. Only integrations with respect to α and β remain to be done:

$$E=\int f^*(\alpha)K(\alpha,\beta)f(\beta)d\alpha d\beta \Big/ \int f^*(\alpha)I(\alpha,\beta)f(\beta)d\alpha d\beta. \quad (24)$$

Here the "overlap integral," I, and the "energy kernel," K, are abbreviations for the expressions

$$\begin{Bmatrix} I(\alpha,\beta) \\ K(\alpha,\beta) \end{Bmatrix} = \int \varphi^*(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha) \begin{Bmatrix} 1 \\ H \end{Bmatrix} \times \varphi(\mathbf{x}_1,\cdots,\mathbf{x}_A;\beta)d^3x_1\cdots d^3x_A, \quad (25)$$

which are Hermitian in the sense

$$I^*(\alpha,\beta)=I(\beta,\alpha), \quad K^*(\alpha,\beta)=K(\beta,\alpha). \quad (26)$$

The generator wave function has now to be chosen to extremize the integral (24):

$$0=\delta E=\frac{\int d\alpha\delta f^*(\alpha)\int d\beta[K(\alpha,\beta)-EI(\alpha,\beta)]f(\beta)d\beta+\text{comp. conj.}}{\int f^*(\alpha)I(\alpha,\beta)f(\beta)d\alpha d\beta}. \quad (27)$$

The coefficients of $\delta f^*(\alpha)$ and $\delta f(\alpha)$ must vanish individually, because these are two linearly independent variations. Thus one arrives at the generator wave equation

$$\int [K(\alpha,\beta)-EI(\alpha,\beta)]f(\beta)d\beta=0, \quad (28)$$

and its complex conjugate which need not be recorded.

The "wave equation" (28) is an integral equation, whereas the Schrödinger equation is conventionally written as a differential equation. The difference is largely formal. The usual Schrödinger equation can also be written as an integral equation by the substitutions

$$I(\alpha,\beta)\to\delta(\beta-\alpha),$$
$$K(\alpha,\beta)\to\frac{\hbar^2}{2\mathfrak{M}}\delta''(\beta-\alpha)+\delta(\beta-\alpha)V\left(\frac{\beta+\alpha}{2}\right), \quad (29)$$

as pointed out long ago by Dirac.[13] He emphasized that the δ-function form of the potential energy part of the kernel is appropriate only in the case where the forces under consideration are velocity independent. In the more general case where the forces depend upon ve-

[13] P. A. M. Dirac, Proc. Cambridge Phil. Soc. **26**, 376 (1930).

locity, he showed that one is naturally led to a more general kernel to represent the potential of the forces.[14] Conversely, one can interpret (28) purely formally to mean that our description of collective motions contains a velocity-dependent effective potential.

Properties of the Generator Wave Function, $f(\alpha)$

Solutions of Eq. (28) which belong to two distinct eigenvalues, E_v and $E_{v'}$, satisfy a generalized condition of orthogonality. To derive this relation, one (1) writes down Eq. (28) for $f_{v'}(\beta)$, (2) multiplies it on the left by $f_v^*(\alpha)$, (3) integrates over α, (4) writes down the corresponding expression with the roles of v and v' interchanged, takes its complex conjugate, and subtracts, using the fact that I and K are Hermitian. One finds the result

$$(E_{v'}-E_v)\int f_v^*(\alpha)I(\alpha,\beta)f_{v'}(\beta)d\alpha d\beta=0, \qquad (30)$$

from which the appropriate definition of orthogonality is at once obvious.

We shall assume that the family of all proper functions, $f_v(\beta)$, is complete in the sense that any continuous function $F(\beta)$ with finite generalized norm,

$$\int\int F^*(\alpha)I(\alpha,\beta)F(\beta)d\alpha d\beta=M<\infty, \qquad (31)$$

can be expressed as a linear combination of these proper functions:

$$F(\beta)=\int\sum_{v=0} C_v f_v(\beta). \qquad (32)$$

Then the coefficients in the expansion are evidently

$$C_v=\int f_v^*(\alpha)I(\alpha,\beta)F(\beta)d\alpha d\beta. \qquad (33)$$

With this expansion, the formal machinery of the method of generator coordinates is completed in its most primitive form. Special ways of solving the wave equation (28) are summarized in Table III and discussed in the following sections.

The ground-state eigenfunction, $f_0(\alpha)$, in the examples that we have considered has qualitatively the character of the lowest eigenfunction of the harmonic oscillator problem. The spread, Δx, in that familiar problem of Schrödinger wave mechanics is determined by the balance between kinetic and potential energy:

$$E\sim\frac{\hbar^2}{2\mathfrak{M}(\Delta\alpha)^2}+\tfrac{1}{2}\mathfrak{M}\Omega^2(\Delta\alpha)^2=\text{minimum}. \qquad (34)$$

[14] See also J. A. Wheeler, Phys. Rev. **50**, 643 (1936); K. Way and J. A. Wheeler, Phys. Rev. **50**, 675L (1936) and **51**, 552 (1937); L. Eisenbud and E. P. Wigner, Proc. Natl. Acad. Sci. U. S. **27**, 281 (1941); and Blanchard, Avery, and Sachs, Phys. Rev. **78**, 292L (1950) and **79**, 220(A) (1950) for further considerations on velocity-dependent forces.

In the present problem of collective motions, it might seem that the kinetic energy is all included already in the basic nucleonic wave function, $\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)$. If that view were correct, there should be no term in the energy that *increases* as the spread, $\Delta\alpha$, is decreased—like the first term in (34). Then the minimum energy would be achieved by making $\Delta\alpha=0$. In other words, the generator function, $f(\alpha)$, would become a δ function centered on some still undetermined value of α. Selecting that value of α to minimize the energy would be nothing but the old fashioned optimization of a trial wave function, now the function $\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)$, with respect to one or more conventional variational parameters, α. No trace would remain of any collective motion.

Actually not all of the kinetic energy *is* included in the preliminary nucleonic wave function. Folding that wave function into the generator wave function produces a final wave function, $\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_A)$ with altered kinetic energy. This alteration appears most clearly in Fig. 2, where one sees the extra "collective node" introduced into the final wave function by the folding process. Even for a generator wave function, $f(\alpha)$, that has no nodes, and that resembles a Gaussian function, the kinetic energy *increases* as the spread, $\Delta\alpha$, of the Gaussian is decreased. However, this increase in kinetic energy does not continue without limit as it does in the familiar oscillator problem (Fig. 3). The wave function, $\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)$, has after all a perfectly finite kinetic energy.

The switch from a trial wave function $\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)$ with fixed α to a trial function built by folding φ and f together can at most lower the collective kinetic energy by the amount indicated in Fig. 3. Not even all that improvement is realizable. The collective potential energy increases approximately as $(\Delta\alpha)^2$ in the examples that we have examined. Consequently, there is ordinarily an optimum value of the spread, $\Delta\alpha$, for minimizing the total energy.

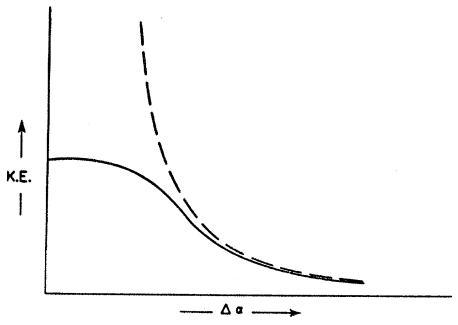

FIG. 3. Kinetic energy associated with collective motion as a function of the spread, $\Delta\alpha$, of the ground state generator wave function, $f(\alpha)$, (qualitative). The dashed curve gives the corresponding kinetic energy for a real oscillator of the same inertial constant, $\mathfrak{M}$. The expectation value of the collective kinetic energy falls off quadratically for small $(\Delta\alpha)^2$, whereas the expectation value of the collective potential energy rises quadratically, One cannot indefinitely lower the total energy by increasing $\Delta\alpha$, however, because the kinetic energy stops falling off as fast as quadratically.

It can happen that the initial falloff of the kinetic energy, also proportional to $(\Delta\alpha)^2$, is characterized by a smaller proportionality constant than the corresponding constant for the rise of the potential energy. In this event, one has to set $\Delta\alpha=0$ to minimize the energy of the system. One example of this kind showed itself in the calculations reported in the following paper on spheroidal deformations of O^{16}, in the special case where large strength constants were assumed for the two-body forces in the original Hamiltonian. No such difficulty appeared for weaker strength constants or for either choice of strength constants in the case of dilatational oscillations. In those cases, the use of a ground state generator wave function, $f(\alpha)$, of optimum spread lowered the total energy of the system by amounts of the order of $\frac{1}{4}$ Mev.

At this point, there appears more clearly than ever the distinction between the parameter, α, that measures the deformation of the generator potential and a real collective coordinate, $\xi(\mathbf{x}_1,\cdots\mathbf{x}_A)$, that measures, for example, the fractional dilatation of the particles in the nucleus. A zero value for $\Delta\alpha$ by no means implies a zero value for the spread, $\Delta\xi$, in values of the collective coordinate. That spread has a certain natural minimum value, $(\Delta\xi)_{\min}$, for the preliminary nucleonic wave function, $\varphi(\mathbf{x}_1,\cdots,\mathbf{x}_A;\alpha)$. To fold this function into a generator wave function of spread, $\Delta\alpha$, is, qualitatively speaking, to increase the spread of ξ in the final-system wave function to something roughly of the form

$$\Delta\xi=[(\Delta\xi)_{\min}{}^2+\text{const}(\Delta\alpha)^2]^{\frac{1}{2}}. \tag{35}$$

If the optimum spread in $\Delta\xi$ is greater than $(\Delta\xi)_{\min}$, the increase is easily arranged by the method of generator coordinates. If the optimum spread is less than $(\Delta\xi)_{\min}$, one may go back to the construction of the original nucleonic wave function and look for a means to construct a wave function of smaller spread, $(\Delta\xi_{\min})$. Or it is conceivable that the method of generator coordinates is not adapted to analyzing collective motions of the presumed symmetry. Or it may be more natural to conclude that the system does not exhibit this particular type of collective motion.

This analysis of relative spreads in ξ and in α furnishes some background for an alternative formalism that we have not found worth pursuing. One can look for a way to put the normalization integral in a more conventional form. One can transform from the generator wave function, $f(\alpha)$, to a new function, g, of a new variable, η, in such a way that

$$\int\int f_v{}^*(\alpha)I(\alpha,\beta)f_{v'}(\beta)d\alpha d\beta=\int g_v{}^*(\eta)g_{v'}(\eta)d\eta. \tag{36}$$

For this purpose, one defines a "broadening kernel," $B(\eta,\beta)$, and its reciprocal, a "narrowing kernel," $N(\beta,\eta)$, as follows:

$$\begin{aligned}&\int N^*(\alpha,\eta)d\alpha I(\alpha,\beta)d\beta N(\beta,\eta')=\delta(\eta-\eta'),\\&\int B(\eta,\beta)d\beta N(\beta,\eta')=\delta(\eta-\eta'),\\&\int N(\alpha,\eta)d\eta B(\eta,\beta)=\delta(\alpha-\beta).\end{aligned} \tag{37}$$

Then the old and new generator wave functions are connected by the relations

$$\begin{aligned}f_v(\beta)&=\int N(\beta,\eta)g_v(\eta)d\eta,\\g_v(\eta)&=\int B(\eta,\beta)f_v(\beta)d\beta.\end{aligned} \tag{38}$$

The energy kernel, $K(\alpha,\beta)$ is transformed to the new energy kernel,

$$L(\eta,\eta')=\int N^*(\alpha,\eta)d\alpha K(\alpha,\beta)d\beta N(\beta,\eta'). \tag{39}$$

The transformed generator wave equation takes the form

$$\int L(\eta,\eta')g_v(\eta')d\eta'=E_v g(\eta). \tag{40}$$

In the particularly simple case (Sec. III) when the overlap kernel has the form

$$I(\alpha,\beta)=\exp[-s(\beta-\alpha)^2],$$

we evaluate the broadening and narrowing kernels with the results

$$N(\beta,\eta)=(\text{const})\int dq\,\exp[(q^2/8s)+iq(\beta-\eta)]$$

(the integration over q is to be carried out after the integration over η) and

$$B(\eta,\beta)=(\text{const})\,\exp[-2s(\eta-\beta)^2]. \tag{41}$$

Of course, a function $g(\eta)$ that is already narrow cannot be further narrowed. In mathematical terms, the integral (40) for $f(\beta)$ will not converge unless the Fourier transform of $g(\eta)$ falls off fast enough at high wave numbers. These features of narrowing and broadening suggest that the new variable η just defined may be closely related to the true collective variable ξ.

Inclusion of Nucleonic Excitations in Analysis

So far, we have considered collective states of motion built upon the lowest nucleonic state of the system. When both nucleonic and collective motions are ex-

cited, it is natural to consider a trial wave function of the form

$$\Psi(\mathbf{x})=\sum_n \int \varphi_n(\mathbf{x};\alpha) f^{(n)}(\alpha) d\alpha. \quad (42)$$

Then straightforward application of the variational principle leads to the conclusion that the coefficient of every $\delta f^{(m)*}(\alpha)$ must vanish in the expression for δE. In this way, one arrives at a series of coupled wave equations ($m=0, 1, 2, \cdots$) for the generator wave functions, $f^{(n)}(\beta)$:

$$\sum_n \int [K_{mn}(\alpha,\beta)-EI_{mn}(\alpha,\beta)] f^{(n)}(\beta) d\beta=0. \quad (43)$$

Here the overlap and energy kernels have the values

$$\begin{Bmatrix} I_{mn}(\alpha,\beta) \\ K_{mn}(\alpha,\beta) \end{Bmatrix} = \int \varphi_m^*(\mathbf{x};\alpha) \begin{Bmatrix} 1 \\ H \end{Bmatrix} \times \varphi_n(\mathbf{x};\beta) d^3x_1 \cdots d^3x_A. \quad (44)$$

Obviously the system of equations (43) is difficult to analyze. It is one simplification that the off-diagonal overlap kernels vanish when $\alpha=\beta$. This circumstance suggests the crude approximation of neglecting both overlap *and* Hamiltonian off-diagonal kernels altogether. In this approximation, states of collective excitation are built upon states of nucleonic excitation without any allowance whatever for interchange of energy between the two kinds of excitation. The system of equations (43) then breaks apart into separate equations of the type that we have already considered. The typical solution may be designated by the symbol $f_v^{(n)}(\beta)$. On being folded into the nucleonic state $\varphi_n(\mathbf{x};\alpha)$ it gives a system wave function $\Psi_{nv}(\mathbf{x})$ with the expectation value E_{nv} for the energy.

In an improved approximation, one can allow in appropriate cases for the coupling between collective and intrinsic excitations, particularly in situations where radiationless transitions between neighboring energy surfaces become important.[15]

Nothing said so far establishes any well-defined way to go on improving indefinitely the degree of approximation to an accurate solution. The expansion (42) is far from unique. Let α be fixed. Then the infinite series of functions $\varphi_n(\mathbf{x};\alpha)$ is already a complete set in terms of which the accurate solution can be expanded. The same is true if α is fixed at another value. There is, therefore, a great arbitrariness in the choice of the functions $f^{(n)}(\alpha)$ in the expansion (42). The same conclusion can be stated in other terms. The set of functions $\Psi_{n,v}(\mathbf{x}_1,\cdots\mathbf{x}_A)$ is formally *over-complete*. To get a complete set of functions, it would seem sufficient to fix v once and for all and to assign all values to the set of nucleonic quantum numbers, n. To let v take on the values $0, 1, \cdots$ is to overpopulate the basis state functions many times over.

The expansion of the accurate state function $\Psi(\mathbf{x})$ in terms of nucleonic wave functions $\varphi_n(\mathbf{x};\alpha)$ for a *fixed* value, $\alpha=\alpha_0$, though possible in principle, is inappropriate in practice. Such an expansion demands that one go to very high states of excitation of the individual nucleons. However, all semblance of collective motion may be expected to disappear at extremely high excitations. The deformation parameter, α, loses its usefulness. Folded wave functions of the type $\Psi_{nv}(\mathbf{x}_1,\cdots\mathbf{x}_A)$ of reasonable excitation will not be able to describe the state of the system to any acceptable approximation. The number of acceptable state functions available for expansion purposes, far from being overcomplete, may well not even be numerous enough for completeness.

This incompleteness of the quantum-mechanical description of collective motion is accepted here, not as an unhappy consequence of a deficient mathematical framework, but as a natural and expected consequence of the very nature of collective motion. There is a fundamental contrast between collective vibrations and rotations on the one hand, and collective translation on the other. In the case of translation, the law of conservation of linear momentum guarantees the existence of a useful center-of-mass coordinate. In the case of rotation, there exists a law of conservation of angular momentum, of course, but it provides no integrable relation among the nucleonic coordinates. Any coordinate for collective rotation derives its usefulness, not from the law of conservation of angular momentum, but from the definability of the nuclear surface. The same is true of typical deformation coordinates. But this definability is approximate only. It is washed out more and more at higher and higher excitations. The collective coordinates are not in principle separable. Consequently, one ought not to expect a well-defined partition of the Hamiltonian into a collective and an intrinsic part. One should be content if the approximate character of the variational method corresponds to the limit definability of the collective motion. If these considerations make one modest in his demands for a description of collective motions, then the method of generator coordinates may satisfy part of these demands.

III. QUADRATIC APPROXIMATION

Origin of the Quadratic or Gaussian Approximation

We consider here the case where the overlap kernel can be well approximated by a Gaussian function of the form

$$I(\alpha,\beta)=\exp[-s(\beta-\alpha)^2], \quad (45)$$

and where the ratio of kernels, K/I, is a simple quadratic function of β and α as indicated in Eq. (10).

It is reasonable to expect a Gaussian behavior for $I(\alpha,\beta)$ when (1) the number of particles is very large

[15] Reference 10, Figs. 24, 25, 33, and 34.

and (2) the nucleonic wave function is well represented by a Slater determinant of the form

$$\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)=\begin{vmatrix} u_1(\mathbf{x}_1,\alpha)&\cdots u_1(\mathbf{x}_A,\alpha)\\ \vdots&\vdots\\ u_A(\mathbf{x}_1,\alpha)\cdots u_A(\mathbf{x}_A,\alpha)\end{vmatrix}. \quad (46)$$

Then the overlap integral has the form

$$I(\alpha,\beta)\equiv\int\varphi^*(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)\varphi(\mathbf{x}_1,\cdots\mathbf{x}_A;\beta)d\mathbf{x}_1\cdots d\mathbf{x}_A$$
$$=\begin{vmatrix}(\alpha,\beta)_{11}\cdots(\alpha,\beta)_{1A}\\ \vdots\quad\quad\vdots\\ (\alpha,\beta)_{A1}\cdots(\alpha,\beta)_{AA}\end{vmatrix}, \quad (47)$$

where the typical one-particle matrix element has received the abbreviation

$$(\alpha,\beta)_{ik}=\int u_i^*(x,\alpha)u_k(x,\beta)dx. \quad (48)$$

This matrix element has the value

$$(\alpha,\alpha)_{ik}=\delta_{ik}, \quad (49)$$

when the deformation parameters are the same for both nucleonic states. When the two deformation parameters differ by the small amount

$$\delta=\beta-\alpha, \quad (50)$$

then diagonal elements have the form

$$(\alpha,\beta)_{kk}=1-a_k\delta^2+\cdots. \quad (51)$$

Here $a_k(\gamma)$ is a slowly varying real positive function of the mean deformation coordinate

$$\gamma=(\alpha+\beta)/2. \quad (52)$$

Off-diagonal elements have the form

$$(\alpha,\beta)_{ik}=a_{ik}\delta+\cdots, \quad (53)$$

where the numbers $a_{ik}(\gamma)$ form an anti-Hermitian matrix. Thus the overlap integral in lowest approximation takes the form[16]

$$I(\alpha,\beta)=\begin{vmatrix}(1-a_1\delta^2)&a_{12}\delta&\cdots&a_{1n}\delta\\ -a_{12}{}^*\delta&(1-a_2\delta^2)\cdots&&a_{2n}\delta\\ \vdots&\vdots&\cdots&\vdots\\ -a_{1n}{}^*\delta&-a_{2n}{}^*\delta&\cdots&(1-a_n\delta^2)\end{vmatrix}$$
$$\approx 1-(\sum_i a_i-\sum_{i<k}|a_{ik}|^2)\delta^2+\cdots. \quad (54)$$

The coefficient of δ^2 is easily seen to be positive definite; the projection of one state on a different state always has a modulus less than unity. One is accustomed to expressing the product of many factors that are nearly equal to one

$$(1-\epsilon_1)(1-\epsilon_2)\cdots(1-\epsilon_n), \quad (55)$$

in the form

$$\exp(-\epsilon_1-\epsilon_2\cdots-\epsilon_n), \quad (56)$$

which is known to give a very good approximation to the same result. No way is evident to generalize the argument from a product to a determinant. We have not found an argument to prove that I should be well represented by the formula

$$I(\alpha,\beta)\approx\exp[-(\sum_i a_i-\sum_{i<k}|a_{ik}|^2)\delta^2], \quad (57)$$

so long as every individual correction factor, $a_i\delta^2$ and $a_{ik}\delta$, is small compared to one, no matter how large the number of particles is made. However, numerical calculations for the case of 16 particles bound in a deformable harmonic-oscillator potential (next article) show that the Gaussian error function approximation fits the computed values of I to 10 percent over a range of I values extending from 1.00 down to 0.03, and much better over most of the range. Consequently, we conclude that it is reasonable to approximate the overlap kernel by a Gaussian error function of the difference, $\delta=\beta-\alpha$.

As for the dependence of $I(\alpha,\beta)$ upon the mean deformation, $\gamma=\frac{1}{2}(\alpha+\beta)$, we know that $I=1$ for $\delta=0$, whatever be the value of γ. Consequently, we adopt the simplest assumption and take I to be independent of γ for *all* values of the difference, $\delta=\beta-\alpha$:

$$I=\exp[-s(\beta-\alpha)^2]. \quad (58)$$

The Hamiltonian kernel,

$$K(\alpha,\beta)=\int\varphi^*(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)\Big[\frac{\mathbf{p}_1{}^2}{2m}+\cdots+\frac{\mathbf{p}_A{}^2}{2m}$$
$$+\sum_{i<k}V(r_{ik})\Big]\varphi(\mathbf{x}_1,\cdots,\mathbf{x}_A;\beta)d\mathbf{x}_1\cdots d\mathbf{x}_A, \quad (59)$$

is most easily analyzed in the case where the difference $\delta=\beta-\alpha$ is zero. Then it represents the expectation value of the energy for a wave function endowed with one or more variational parameters, α. This energy must exhibit a minimum if (1) the system is endowed with stability with respect to deformations of the type in question and (2) the nucleonic trial wave function is well adapted to recognizing this stability. Let these conditions be satisfied. Let the point of equilibrium be placed at $\alpha=\beta=0$ by suitable definition of these deformation coordinates. Let the expectation value of the energy be developed in a power series about this equilibrium point through terms of the second order in

[16] Reference 10 gives this analysis for the case of particles bound in a one-dimensional square potential well. There the diagonal coefficients have the value $a_j=\frac{1}{8}+(j^2\pi^2/6)$, and the off-diagonal coefficients are $a_{jk}=(-1)^{j+k}2jk/(j^2-k^2)$. The coefficient, $\{\Sigma a_j-\Sigma_{j<k}|a_{jk}|^2\}$, of $-\delta^2$ in (54) has for large values of n the approximate value $(n/4)+(41/288)+(12)^{-1}(6n^2+6n+1)\times\ln(3.562n)$, as seen in the following listing:

n		2	3	4	5
Coefficient of $-\delta^2$ from	accurate summation	6.6969	15.3038	27.9304	44.8293
	asymptotic formula	6.6964	15.3034	27.9299	44.8287

See also M. G. Redlich and E. P. Wigner, Phys. Rev. **95**, 122 (1954) for the analogous problem for a three-dimensional square well.

$\gamma=\frac{1}{2}(\alpha+\beta)=\alpha=\beta$; thus,

$$K(\alpha,\beta)=K(\gamma-\tfrac{1}{2}\delta,\ \gamma+\tfrac{1}{2}\delta)_{\delta=0}$$
$$=K(\gamma,\gamma)=K_0+\tfrac{1}{2}\mathfrak{M}\Omega^2\gamma^2+\cdots. \quad (60)$$

Now fix $\gamma=\frac{1}{2}(\alpha+\beta)$ and change $\delta=\beta-\alpha$. For large values of δ, the two deformations $\alpha=\gamma-\frac{1}{2}\delta$ and $\beta=\gamma+\frac{1}{2}\delta$ differ substantially. The value of the Hamiltonian kernel will be dominated by the decreasing overlap of the two nucleonic wave functions. To recognize this effect, we consider the quotient K/I. The Hamiltonian is Hermitian. Consequently, K, I and their quotient are all even functions of δ. Therefore, we can express the ratio in a power series in δ good through terms of the third order in the form

$$K/I=\text{constant}+\text{constant}\ \delta^2+\tfrac{1}{2}\mathfrak{M}\Omega^2\gamma^2$$
$$=E_g+\frac{\hbar^2}{2\mathfrak{M}}[2s-4s^2(\beta-\alpha)^2]+\tfrac{1}{2}\mathfrak{M}\Omega^2\left(\frac{\beta+\alpha}{2}\right)^2. \quad (61)$$

The qualitative dependence of the ratio of kernels, K/I, upon the deformation parameters is shown in perspective in Fig. 4.

In the following paper, the Hamiltonian kernel is computed explicitly for a simple treatment of collective motions in O^{16}. It is found there that the quadratic form (61) provides a good representation of the ratio of kernels over the range of deformations of interest. Consequently, we believe that the quadratic approximation is useful for an appreciable range of problems.

Solution of the Generator Wave Equation for Quadratic Kernels

In this quadratic approximation, the generator wave equation,

$$\int[K(\alpha,\beta)-E_vI(\alpha,\beta)]f_v(\beta)d\beta=0, \quad (62)$$

on division by $\frac{1}{2}\hbar\Omega$, takes the *harmonic-oscillator form*

$$\int\{(\hbar/\mathfrak{M}\Omega)[2s-4s^2(\beta-\alpha^2)]+(\mathfrak{M}\Omega/\hbar)[\tfrac{1}{2}(\beta+\alpha)]^2$$
$$-2(E_v-E_g)/\hbar\Omega\}\exp[-s(\beta-\alpha)^2]f_v(\beta)d\beta=0. \quad (63)$$

We can try a solution of the form

$$f_0(\beta)=N_0\exp(-\beta^2/2a^2), \quad (64)$$

where a is a constant so far undetermined. Then the integrals in (63) are easily computed explicitly, with the result that the equation takes the form

$$(\pi/s)^{\frac{1}{2}}[1+(2sa^2)^{-1}]^{-\frac{1}{2}}$$
$$\times[g_1(\mathfrak{M}\Omega/\hbar s,sa^2)-2(E_0-E_g)/\hbar\Omega+g_2(\mathfrak{M}\Omega/\hbar s,sa^2)s\alpha^2]$$
$$\times\exp[-s\alpha^2/(1+2sa^2)]=0, \quad (65)$$

where

$$g_1(u,v)=\binom{2}{u}\left[1-\frac{1-\frac{1}{16}u^2}{1+(2v)^{-1}}\right] \quad (66)$$

and

$$g_2(u,v)=\binom{4}{u}[1+u^2]\left[\frac{1}{1+(2v)^{-1}}-\frac{1+\frac{1}{4}u}{1-\frac{1}{4}u}\right]$$
$$\times\left[\frac{1}{1+(2v)^{-1}}-\frac{1-\frac{1}{4}u}{1+\frac{1}{4}u}\right]. \quad (67)$$

The curly brackets in Eq. (63) contain one constant term and one term proportional to α^2, both of which must vanish. These two conditions determine the unknown energy and spread of the ground-state wave

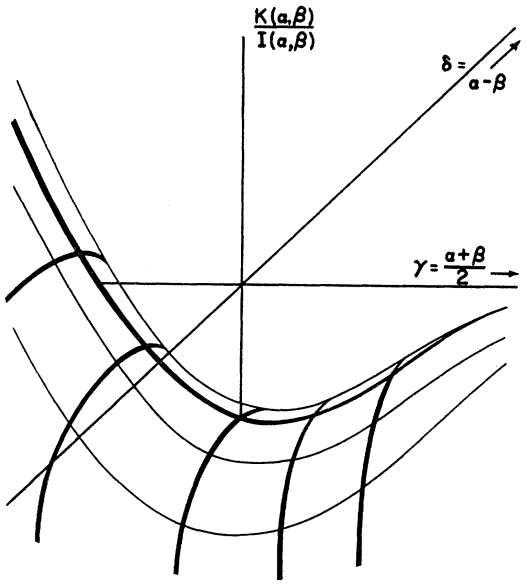

FIG. 4. Qualitative dependence of the ratio of kernels, $K(\alpha,\beta)/I(\alpha,\beta)$, upon the deformation parameters. The expectation value of the energy is governed by the balance of two effects: the rise in K in the δ direction, physically to be understood as an increase in potential energy; and the fall of K in the δ direction, to be interpreted as decrease of kinetic energy. When the generator wave function has a Gaussian form, $f(\alpha)=\exp(-\alpha^2/2a^2)$, the typical value of K is weighted by the factor $f(\alpha)f(\beta)$; that is, by a circularly symmetric weighting factor. The larger the radius of this probability distribution, the higher would be the expectation value of the energy if the positive curvature of K/I in the γ direction exceeded the negative curvature of K/I in the δ direction. In this anomalous case, the energy of the system is obviously optimized by a probability distribution of zero spread. In the normal case, the fall off in the δ direction dominates, and the energy is lowered by attributing a finite radius to the probability distribution. If one radius for the distribution lowers the energy, will not a radius twice as great produce four times the lowering in the energy? Yes, for small radii. No, for large radii. The quantity being weighted is not K/I, but K itself, which contains the extra factor $I=\exp(-s\delta^2)$. This circumstance means that one cannot go on lowering the kinetic energy indefinitely by an amount proportional to the square of the spread in f. This feature of the expectation value of the kinetic energy shows up in Fig. 3. It implies that there exists a well-defined optimum spread in $f(\alpha)$ for maximum reduction in the energy of the system.

function

$$E_0=E_g+\tfrac{1}{2}\hbar\Omega-(\mathfrak{M}\Omega^2/16s),$$
$$a^2=(\hbar/\mathfrak{M}\Omega)-(1/4s). \tag{68}$$

The zero-point energy above the constant energy E_g has the familiar value $\frac{1}{2}\hbar\Omega$ in the limiting case, $s\rightarrow\infty$, of an overlap kernel of very narrow spread. When the spread has the maximum allowable value, and $s=\mathfrak{M}\Omega/4\hbar$, then the zero-point energy above E_g is only half as great: $\frac{1}{4}\hbar\Omega$.

In a similar way, one verifies that

$$E_1=E_g+\tfrac{3}{2}\hbar\Omega-(\mathfrak{M}\Omega^2/16s),$$
$$f_1(\beta)=N_1\beta\exp(-\beta^2/2a^2), \tag{69}$$

also satisfy the generator wave equation.

Wave functions for higher excited states can be expressed in the form

$$f_v(\beta)=N_vP_v(\beta/a)\exp(-\beta^2/2a^2), \tag{70}$$

where the vth order polynomial $P_v(x)$, is *not* ordinarily a Hermite polynomial. Instead, it is given by the recursion formula

$$P_v(x)=(x+Ad/dx)P_{v-1}(x), \tag{71}$$

where

$$A=-\tfrac{1}{2}-(\mathfrak{M}\Omega/8\hbar s). \tag{72}$$

The corresponding energy values are

$$E_v=E_g+(v+\tfrac{1}{2})\hbar\Omega-(\mathfrak{M}\Omega^2/16s). \tag{73}$$

Thus the harmonic oscillator is almost as easy to treat within the scheme of the integral equation (9) as in the familiar Schrödinger formalism.

IV. CORRESPONDENCE BETWEEN INTEGRAL EQUATION AND SCHRÖDINGER DIFFERENTIAL EQUATIONS; δ-FUNCTION APPROXIMATION

Quadratic Kernels in the Limit of Small Spread

When (1) the spread of the overlap kernel becomes very small and (2) this kernel is adequately represented by a δ function, the integral equation (28) transforms into the Schrödinger equation. Beginning with the case of the harmonic oscillator, set equal to infinity the quantity s that measures the reciprocal of the square of the spread of the Gaussian error type of kernel, I. Then the spread constant, a^2, for the ground-state wave function itself (68) goes to the familiar Schrödinger value

$$a^2\rightarrow\hbar/\mathfrak{M}\Omega. \tag{74}$$

Similarly, the recursion formula (71) for constructing excited-state wave functions goes to the Hermite form

$$H_v(x)=(x-\tfrac{1}{2}d/dx)H_{v-1}(x). \tag{75}$$

For a closer view of the transition to a differential equation, write the integral equation in the form

$$\int[K_{\rm norm}(\alpha,\beta)-E_vI_{\rm norm}(\alpha,\beta)]f_v(\beta)d\beta=0, \tag{76}$$

where

$$I_{\rm norm}=(s/\pi)^{\frac{1}{2}}I=(s/\pi)^{\frac{1}{2}}\exp[-s(\beta-\alpha)^2], \tag{77}$$

and

$$K_{\rm norm}=(s/\pi)^{\frac{1}{2}}K. \tag{78}$$

In the limit $s\rightarrow\infty$,

$$I_{\rm norm}\rightarrow\delta(\beta-\alpha) \tag{79}$$

and

$$K_{\rm norm}=K_{\rm const}+K_{\rm pot\ norm}+K_{\rm kin\ norm}, \tag{80}$$

with

$$K_{\rm const\ norm}=E_gI_{\rm norm}(\alpha,\beta)\rightarrow E_g\delta(\beta-\alpha); \tag{81}$$

$$K_{\rm pot\ norm}=\tfrac{1}{2}\mathfrak{M}\Omega^2\left(\frac{\beta+\alpha}{2}\right)^2I_{\rm norm}(\alpha,\beta)$$
$$\rightarrow\tfrac{1}{2}\mathfrak{M}\Omega^2\left(\frac{\beta+\alpha}{2}\right)^2\delta(\beta-\alpha) \tag{82}$$

and

$$K_{\rm kin\ norm}(\alpha,\beta)=(\hbar^2/2\mathfrak{M})(s/\pi)^{\frac{1}{2}}$$
$$\times[2s-4s^2(\beta-\alpha)^2]\exp[-s(\beta-\alpha)^2]$$
$$\rightarrow-(\hbar^2/2\mathfrak{M})\delta''(\beta-\alpha). \tag{83}$$

Evidently the integral equation goes over in this limit to the familiar Schrödinger form

$$-(\hbar^2/2\mathfrak{M})f''(\alpha)+E_gf(\alpha)$$
$$+\tfrac{1}{2}\mathfrak{M}\Omega^2\alpha^2f(\alpha)-E_vf(\alpha)=0, \tag{84}$$

as expected.

δ-Function Limit for Kernels That Are Not Quadratic

We have identified the δ-dependent part of the energy kernel, $K(\alpha,\beta)$, with a kinetic-energy operator and the γ-dependent part with potential energy. This possibility of this decomposition will not be expected to disappear when the dependence of the potential energy upon the mean deformation parameter, $\gamma=\frac{1}{2}(\alpha+\beta)$, is no longer quadratic. One will still expect to approximate the δ dependence of the kernel by a Dirac δ'' function in the case where K is appreciable for only a small range of δ. This limiting situation will be expected when the number of nucleons is exceedingly large. The coefficient of the δ'' factor will, in general, be γ-dependent. In other words, the effective inertial constant of the collective motion will depend upon the deformation.[17] The generator wave equation in this limit will still go over to a differential equation, but a differential equation of the form

$$(d/d\alpha)[\hbar^2/2\mathfrak{M}(\alpha)](df/d\alpha)+[E_v-V(\alpha)]f(\alpha)=0. \tag{85}$$

This approximation is appropriate when we neglect the velocity dependence of the potential energy and of the inertial parameters of the collective motion.

[17] S. Moszkowski, Phys. Rev. **103**, 1328 (1956).

V. DIFFICULTY OF THE EFFECTIVE MASS

Idealized Problem of Two Particles in One Dimension as an Example; Harmonic Oscillator Construction Potential

In the analysis of collective motions both in the quadratic approximation (Sec. III) and in the δ-function approximation (Sec. IV), there came into evidence in a very natural way an inertial parameter, $\mathfrak{M}$. To make a simple test of the calculated value of $\mathfrak{M}$ consider a system composed of two particles free to move only along the x-axis, interacting with a short range attractive potential $v(x_2-x_1)$. We shall demand that the wave function be antisymmetric in the coordinates of the two particles.

In the usual method of analysis, one introduces the usual center-of-mass coordinate $X=\frac{1}{2}(x_1+x_2)$ and the relative coordinate $x=x_2-x_1$, separates variables, and finds a solution of the form

$$\Psi(x_1,x_2)=u(x)\exp(ikX), \tag{86}$$

belonging to the energy

$$E=\epsilon+\hbar^2k^2/4M, \tag{87}$$

where $u(x)$ satisfies the equation

$$-(\hbar^2/M)d^2u/dx^2+v(x)u=\epsilon u. \tag{88}$$

This separation of variables is not possible for most collective motions of a nucleus. Consequently, let us start over again and proceed by the method of generator coordinates.

We first introduce the harmonic oscillator construction potential,

$$V(x,\alpha)=\tfrac{1}{2}M\omega^2(x-\alpha)^2, \tag{89}$$

with a strength $\frac{1}{2}M\omega^2$ to be adjusted later. The quantity α is the generator coordinate. We determine the familiar single particle eigenfunctions in this potential and from them we construct the antisymmetrized nucleonic wave function

$$\begin{aligned}\varphi(x_1,x_2;\alpha)&=2^{-\frac{1}{2}}\begin{vmatrix}u_1(x_1;\alpha) & u_1(x_2;\alpha)\\ u_2(x_1;\alpha) & u_2(x_2;\alpha)\end{vmatrix}\\ &=\pi^{-\frac{1}{2}}(M\omega/\hbar)(x_1-x_2)\\ &\times\exp\{-(M\omega/2\hbar)[(x_1-\alpha)^2+(x_2-\alpha)^2]\}.\end{aligned} \tag{90}$$

Next we introduce an as yet undetermined function $f(\alpha)$ and construct the trial system wave function,

$$\Psi(x_1,x_2)=\int\varphi(x_1,x_2;\alpha)f(\alpha)d\alpha. \tag{91}$$

The overlap kernel I and the energy kernel K are given by the formulas

$$\begin{Bmatrix}I(\alpha,\beta)\\ K(\alpha,\beta)\end{Bmatrix}=\int\int\varphi(x_1,x_2;\alpha)\times\begin{Bmatrix}1\\ -(\hbar^2/2M)(\nabla_1^2+\nabla_2^2)+v(x_1-x_2)\end{Bmatrix}\varphi(x_1,x_2;\beta)dx_1dx_2. \tag{92}$$

The integrations over x_1 and x_2 are most simply performed by use of the center-of-mass and relative coordinates, X and x, and the transformation $\nabla_1^2+\nabla_2^2=\frac{1}{2}\nabla_X^2+2\nabla_x^2$. The nucleonic wave function takes the form

$$\pi^{-\frac{1}{2}}(M\omega/\hbar)x\times\exp[-(M\omega/\hbar)(X-\alpha)^2-(M\omega/4\hbar)x^2]. \tag{93}$$

The integrations give for the overlap and energy kernels the expressions

$$\begin{Bmatrix}I(\alpha,\beta)\\ K(\alpha,\beta)\end{Bmatrix}=\begin{Bmatrix}1\\ \epsilon^*+\frac{1}{4}\hbar\omega[1-(M\omega/\hbar)(\beta-\alpha)^2]\end{Bmatrix}\times\exp[-(M\omega/2\hbar)(\beta-\alpha)^2]. \tag{94}$$

Here ϵ^* is the expectation value of the energy of relative motion, calculated for a harmonic-oscillator type of wave function, with node where the particles come together because of the assumed Fermi statistics:

$$\epsilon^*=2\pi^{-\frac{1}{2}}\left(\frac{M\omega}{2\hbar}\right)^{\frac{3}{2}}\int x\exp\left(-\frac{M\omega x^2}{4\hbar}\right)\times\left[-\left(\frac{\hbar^2}{M}\right)\frac{d^2}{dx^2}+v(x)\right]x\exp\left(-\frac{M\omega x^2}{4\hbar}\right)dx. \tag{95}$$

The energy ϵ^* must be a minimum. This type of problem is familiar. No further details need be added.

The solution of the generator Eq. (28) for the collective wave function, $f(\alpha)$, is greatly simplified in the present problem by the circumstance that the kernels $I(\alpha,\beta)$ and $K(\alpha,\beta)$ depend on the difference, $\beta-\alpha$, but not upon α and β individually. This invariance, by well-known group theoretic arguments, leads one to expect solutions corresponding to irreducible representations of the translation group, of the form

$$f(\beta)=\exp(ik\beta), \tag{96}$$

as one also easily checks from (28). The energy has the value

$$\begin{aligned}E&=\int K(0,\beta)\exp(ik\beta)d\beta\Big/\int I(0,\beta)\exp(ik\beta)d\beta\\ &=\epsilon^*+\hbar^2k^2/4M,\end{aligned} \tag{97}$$

where the kinetic energy of collective motion comes into evidence in a straightforward and reasonable way.

This simple result follows from the form of the system wave function. On folding $f(\alpha)=e^{ik\alpha}$ into $\varphi(x_1,x_2;\alpha)$ and omitting an irrelevant multiplicative factor, $(\pi\hbar/M\omega)^{\frac{1}{2}}\exp(-\hbar k^2/4M\omega)$, we find that this system wave function reduces to the product

$$\Psi(x_1,x_2)=\text{const}\times\exp(-M\omega x^2/4\hbar)\exp(ikX)$$

of a well-determined internal wave function and a factor that describes motion of the center of mass.

Two-Particle Problem with a Square Well Construction Potential

No such acceptable result will emerge when we use a nonharmonic construction potential to define the preliminary nucleonic wave function, as was already pointed out by Peierls and Yoccoz.[2] To bring out explicitly the difference, we consider a square well. The individual particle wave functions will have the form

$$\begin{aligned}u_1(x;\alpha)&=(2/L)^{\frac{1}{2}}\cos[\pi(x-\alpha)/L],\\ u_2(x;\alpha)&=(2/L)^{\frac{1}{2}}\sin[2\pi(x-\alpha)/L]\end{aligned}\tag{98}$$

between the limits $x=\alpha-\frac{1}{2}L$ and $x=\alpha+\frac{1}{2}L$, and will vanish outside. The resulting antisymmetrized nucleonic wave function can be expressed in center-of-mass and relative coordinates in the form

$$\varphi(x_1,x_2;\alpha)=\left(\frac{2^{\frac{3}{2}}}{L}\right)\left\{\cos\left[\frac{2\pi(X-\alpha)}{L}\right]+\cos\left(\frac{\pi x}{L}\right)\right\}\times\sin\left(\frac{\pi x}{2L}\right)\cos\left[\frac{\pi(X-\alpha)}{L}\right].\tag{99}$$

The new kernels $I(\alpha,\beta)$ and $K(\alpha,\beta)$ still depend only on the difference, $\beta-\alpha$. Therefore, group theory again says that the generator wave function $f(\beta)=\exp(ik\beta)$ solves the generator wave equation. The energy has as before the form (97), with one part representing internal energy and the other part representing kinetic energy of motion of the center of mass. However, *this internal energy is now dependent upon the wave number, k*:

$$\epsilon^*(k)=(\hbar^2\pi^2/4ML^2)\frac{\pi N_1+N_2\sin\kappa\pi}{\pi D_1+D_2\sin\kappa\pi},\tag{100}$$

where $\kappa=kL/\pi$ and where N_i and D_i are algebraic functions of κ:

$$\begin{aligned}&N_1=\textstyle\sum_i\frac{1}{2}A_i^2a_i^2;\quad D_1=\sum_i\frac{1}{2}A_i^2;\\ &N_2=-\tfrac{1}{2}\textstyle\sum(A_i^2a_i)-\sum_{i<j}A_iA_ja_ia_j/(a_i+a_j);\\ &D_2=-\tfrac{1}{2}\textstyle\sum(A_i^2/a_i)-\sum_{i<j}A_iA_j/(a_i+a_j);\\ &a_1=\kappa+2;\quad a_2=\kappa+4;\quad a_3=\kappa-2;\quad a_4=\kappa-4;\\ &A_1=-4/[(\kappa+3)(\kappa-1)];\quad A_2=2/[(\kappa+1)(\kappa+3)];\\ &A_3=4/[(\kappa-3)(\kappa+1)];\quad A_4=-2/[(\kappa-1)(\kappa-3)].\end{aligned}$$

Thus, for example,

$$D_1=4(\kappa^2-1)^{-2}(\kappa^2-9)^{-2}(5\kappa^6-82\kappa^4+365\kappa^2+288);$$

and for $\kappa=0$,

$$\epsilon^*(k)=(8\hbar^2\pi^2/5ML^2),$$

compared with the correct eigenvalue, $\hbar^2\pi^2/ML^2$, for the lowest state of internal motion. The reason for this unexpected result is simple. The system wave function, $\Psi(x_1,x_2)$ formed by folding together $\varphi(x_1,x_2;\alpha)$ (Eq. 99) and $f(\alpha)=\exp(ik\alpha)$ still factors into two parts,

$$\begin{aligned}\Psi(x_1<x_2)=-\Psi(x_2<x_1)&=(\text{normalization factor})\\ \times\exp[ik(\tfrac{1}{2}x_1+\tfrac{1}{2}x_2)]\{&2(\kappa^2-2\kappa-3)^{-1}\sin[\tfrac{1}{2}(\kappa-2)\eta-\tfrac{1}{2}\kappa\pi]\\ &-2(\kappa^2+2\kappa-3)^{-1}\sin[\tfrac{1}{2}(\kappa+2)\eta-\tfrac{1}{2}\kappa\pi]\\ &+(\kappa^2+4\kappa+3)^{-1}\sin[\tfrac{1}{2}(\kappa+4)\eta-\tfrac{1}{2}\kappa\pi]\\ &-(\kappa^2-4\kappa+3)^{-1}\sin[\tfrac{1}{2}(\kappa-4)\eta-\tfrac{1}{2}\kappa\pi]\},\end{aligned}\tag{101}$$

where $\eta=\pi|x_2-x_1|/L$; but the first factor that describes the internal motion is now dependent upon k. Therefore, it is reasonable that the internal energy should also depend upon k.

No such k dependence of the internal energy appeared in the case of the harmonic-oscillator construction potential, because there the internal wave function was independent of k. This independence came about because the nucleonic wave function in that case factored into a term dependent upon $X-\alpha$ alone and a term dependent upon x alone. No such factorization is possible in the case of the nucleonic wave function (99). As a consequence, the rate of oscillation of the first factor in (101) increases with increasing k.

Two Contributions to the Effective Mass

So much for the origin and nature of the k-dependence of the internal energy, ϵ^*; now for its consequences. Expanding ϵ^* in a power series in k through terms of the second order, we can write the expectation value of the total energy of the system, following Peierls and Yoccoz, in the form

$$\begin{aligned}E&=\epsilon^*(k)+\hbar^2k^2/4M\\ &=(\epsilon_0{}^*+0+\tfrac{1}{2}\epsilon_2{}^*k^2+\cdots)+\hbar^2k^2/4M.\end{aligned}\tag{102}$$

From the momentum dependence of the energy, one can define an effective mass,

$$E=(\text{constant})+\hbar^2k^2/2M_{\text{eff}}+\cdots.\tag{103}$$

For the total mass, we obtain a value

$$M_{\text{eff}}=\frac{1}{(1/2M)+\epsilon_2{}^*/\hbar^2},\tag{104}$$

which is *less* than the correct value. *The method of generator coordinates gives for the inertial parameter of the collective motion a value that is too small* in the case of the square-well construction potential, contrary to

TABLE IV. Comparison of number of parameters needed to specify configuration of construction potential with number of inertial parameters.

Construction potential	Inertial parameters
One-dimensional, translatable arbitrary shape: α	M, mass
Two-dimensional, rotatable arbitrary form: α	A, moment of inertia about center of rotation
Three-dimensional, rotatable, symmetric with respect to rotations about a certain axis which can itself change its orientation: α_1, α_2	A, moment of inertia for rotations about axes perpendicular to the symmetry axis; no meaning for rotations about this axis, and corresponding inertial parameter vanishes.

what happens when the nucleonic wave function is built up out of harmonic-oscillator wave functions.

Generalizing from the two-particle problem just considered, we recognize several instances where the proper form for the generator wave function can be deduced directly from group theory:

$f(\alpha)=e^{ik\alpha}$ in order to generate a state of wave number k when α describes a one-dimensional translation of a construction potential;

$f(\alpha)=e^{im\alpha}$ in order to generate a state of rotational quantum number m when α describes the rotation in a plane of an unsymmetric two-dimensional construction potential, $V(x,y;\alpha)$;

$f(\alpha_1,\alpha_2)=Y_{l,m}(\alpha_1,\alpha_2)$ in order to generate a state of rotational quantum numbers, l and m, when α_1 and α_2 describe the orientation in space of a three-dimensional construction potential of axial symmetry. (105)

In all these cases, we can evaluate the expectation value of the energy at once in terms of the relevant group-theory parameter: k; or m; or l and m; etc., as the case may be. Let this expectation value be expanded in a power series in the parameter in question through terms of the second order. Then the coefficients in this expansion define as indicated by Peierls and Yoccoz—an effective mass or inertial parameter (Table IV):

$$\langle E\rangle=\frac{\langle K\rangle}{\langle I\rangle}=\frac{K_0-\frac{1}{2}K_2k^2+\cdots}{I_0-\frac{1}{2}I_2k^2+\cdots}$$
$$=(K_0/I_0)+\tfrac{1}{2}[(K_0I_2-K_2I_0)/I_0^2]k^2 \quad (106)$$
$$=\text{const}+(\hbar^2k^2/2\mathfrak{M}),$$

with

$$\mathfrak{M}=\hbar^2I_0^2/(K_0I_2-K_2I_0). \quad (107)$$

Here the numbers I_n and K_n are obtained as follows: We take the Fourier transforms of the overlap integral and the energy kernel,

$$I(k)=\int I(\delta)\exp(ik\delta)d\delta,$$
$$K(k)=\int K(\delta)\exp(ik\delta)d\delta, \quad (108)$$

(where $\delta=\beta-\alpha$) and develop them in powers of k and give the coefficient of $(-1)^{n/2}k^n/n!$ the name I_n or K_n as the case may be.

Problem of Testing Correctness of Inertial Parameter

(1) What *is* the correct value of the appropriate inertial parameter in more general problems? (2) What value is predicted by the method of generator coordinates? (3) What conditions have to be satisfied for the two values to agree?

In the case of translational motion, there is no doubt as to the correct value of the inertial parameter: it must equal the total mass of the system. In the case of of collective rotations, according to the investigations of Inglis, Bohr and Mottelson, Moszkowski, and others,[9] the correct moment of inertia is calculable from the response of the nucleonic system to a rotating deformed potential well of the kind that is here called a construction potential. According to these authors, one can calculate the moment-of-inertia parameter in either of two equivalent ways, (1) by evaluating the increment, dL, in the angular momentum of the system per unit increment, $d\omega$, in the angular velocity, ω, of the construction potential:

$$\mathcal{I}_{\text{eff}}=dL/d\omega; \quad (109)$$

or (2) by evaluating to second order the increase, ΔE, in the expectation value of the energy of the nucleons due to the rotation of the construction potential:

$$\mathcal{I}_{\text{eff}}=2\Delta E/\omega^2. \quad (110)$$

It should be clearly stated that none of the cited works given an unambiguous way to associate with a given real physical problem a unique construction potential. They and the method of generator coordinates are alike in leaving the choice of generator potential in the realm more of art than of science. But they—and in particular, Inglis—give a unique prescription to determine the inertial parameters for a given choice of construction potential: (1) Calculate the nucleonic wave functions, $\varphi_n(\mathbf{x}_1,\cdots\mathbf{x}_A;\alpha)$ and the corresponding energy levels, E_n, for a fixed configuration, α, of the construction potential. If the construction potential omits all residual nucleonic forces, φ can be represented as a simple determinable combination of individual particle states in a deformed potential. Otherwise, φ is a complicated many-body wave function. The following

analysis applies to either case. (2) Define the operator $P=-i\hbar\partial/\partial\alpha$. (3) Then the correct inertial parameter, as defined in (109) or (110), will be[18]

$$\mathcal{I}_{\text{eff}}=2\sum_{n>0}\left\{\frac{\langle 0|P|n\rangle\langle n|P|0\rangle}{E_n-E_0}\right\}_{\alpha=0}. \qquad (111)$$

This result applies to the lowest nucleonic state of the system. To an excited state, a similar formula applies. It is obtained by making obvious changes in (111).

It should be clearly stated that the inertial parameter (111) is the correct result for the problem of particles in a construction potential of the given form that is translated or rotated or vibrated at a slow and constant rate by external machinery. This is the reason why the formula has a perturbation-theoretical character. A very small perturbation of the boundary conditions couples the initial state 0 to a typical excited state n both states being defined for the *same configuration* of the construction potential.

In contrast, formula (107) for the inertial parameters from the method of generator coordinates depends upon the coupling, $I(\delta)$ and $K(\delta)$, between wave functions for the *same* state, 0, for very *different configurations* of the construction potential. There is no obvious reason why the two expressions for $\mathfrak{M}$ and $\mathcal{I}_{\text{eff}}$ should turn out to be identical. Moreover, the problems where these two parameters appear are really different: there is no external machinery to drive the construction potential in the problem considered in this paper. Nevertheless, it seems reasonable to believe that the value $\mathcal{I}_{\text{eff}}$ of (111) is approximately correct for collective rotations, and to regard any departure of $\mathfrak{M}$ of Eq. (107) from $\mathcal{I}_{\text{eff}}$ as witness to an inaccuracy in the method of generator coordinates. There is plenty of room for such an error in this method for it relies upon a variational approach exclusively. The trial wave function in the method of generator coordinates is designed for simplicity, not for precision.

[18] D. R. Inglis, Phys. Rev. **97**, 701 (1955).

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