Kinetic Energy of Nuclei in the Hartree Model

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In the present note the question of the separation of the kinetic energy of the center of gravity from the total kinetic energy of the nucleus is considered. This separation is necessitated in the calculation of nuclear energy levels by the use of the Hartree method. It is found that under certain conditions the wave function for the whole nucleus in absolute coordinates can be replaced by a product of the same function of the coordinates of the particles relative to the center of gravity and a 1*s* wave function for the center of gravity. These conditions are that oscillator wave functions be used for the individual particles and that the nucleus contain only one partly filled shell in both protons and neutrons with all shells of lower energy quantum number filled. It then follows that the kinetic energy of the nucleus is equal to the value calculated in absolute coordinates minus the energy of a single 1*s* particle.

IN the calculation of the energy levels of light nuclei from the individual particle model (Hartree approximation), it is the usual procedure to use wave functions in which the nuclear particles are coupled to a fixed point (absolute coordinates) rather than to each other. The kinetic energy T of the nucleus calculated with such wave functions will contain the spurious kinetic energy of the center of gravity which must be deducted. For this purpose several authors have replaced the mass M of a single particle by the reduced mass $M(1-1/N)$ where N is the total number of particles in the nucleus.[1] However, such a procedure is correct only for a two particle problem or for the case that all the particles are in the 1*s* shell. It is our purpose in this note to investigate this point in a somewhat more general case. This investigation, we shall find, is greatly facilitated by the fact that the wave functions ordinarily used, i.e., those in an oscillator potential, actually contain the center of gravity only in a trivial factor. By separating off this factor one obtains directly wave functions containing only relative coordinates.

For the oscillator potential

$$U=-U_0+\tfrac{1}{2}M\omega^2r^2, \tag{1}$$

ω being the frequency of a classical oscillator of mass M (proton or neutron mass) in the field U, the individual particle wave functions in absolute coordinates are:

1*s* level $\psi=ce^{-\alpha r^2}$, (2)

2*p* level $\psi=c'(x, y \text{ or } z)e^{-\alpha r^2}$, (2′)

and in general for "energy quantum number"[2] k,

$$\psi=P_{k-1}(x, y, z)e^{-\alpha r^2}. \tag{2''}$$

Here c and c' are normalization constants, P_{k-1} is a polynomial of degree $k-1$ and

$$\alpha=M\omega/2\hbar. \tag{3}$$

For the wave function Ψ of the whole nucleus we may take a product of two antisymmetric (determinantal) wave functions, one for the neutrons and one for the protons, each determinant being constructed from the spin and space wave functions (2) of the individual particles. In all cases the wave function Ψ will contain the factor $e^{-\alpha\sum_1^N r_i^2}$. This factor may easily be transformed into center of gravity coordinates $\mathbf{R}$ and relative coordinates $\boldsymbol{\varrho}_i$ with respect to that point:

$$\mathbf{R}=\sum_1^N \mathbf{r}_i/N \tag{4}$$

and $$\boldsymbol{\varrho}_i(\xi_i, \eta_i, \zeta_i)=\mathbf{r}_i(x_i, y_i, z_i)-\mathbf{R}(X, Y, Z), \tag{5}$$

writing the Cartesian components of the vectors in the brackets. The relative coordinates $\boldsymbol{\varrho}_i$ are of course not independent but fulfill the relation

$$\sum_1^N \boldsymbol{\varrho}_i=0. \tag{6}$$

[1] Cf., e.g., S. Flügge, Zeits. f. Physik **96**, 459 (1936).

[2] By the energy quantum number k we mean the quantum number which defines the energy of a single particle in the oscillator field. For the field (1) this energy is $E=-U_0+\hbar\omega(k+\frac{1}{2})$. The relation between k and the principal and azimuthal quantum numbers, n and l, is $k=2n-l-1$. See H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. **8**, 82 (1936), §32.

From (5) and (6) it follows that

$$e^{-\alpha\Sigma_1^N r_i^2}=e^{-\alpha N R^2}e^{-\alpha\Sigma_1^N \rho_i^2}. \tag{7}$$

We have now to consider the transformation of the determinants in the wave function which remain after the factorization of the gaussian term (7). For the sake of simplicity we shall first consider the case in which, for each kind of particle, the $1s$ shell is complete and the $2p$ shell is partly filled. In this case each determinant will have, in general, the form

$$D(\mathbf{r}_i)=\begin{vmatrix} \alpha_1 & \beta_1 \cdots & x_1\alpha_1 & \cdots & y_1\beta_1 & \cdots \\ \alpha_2 & \beta_2 \cdots & x_2\alpha_2 & \cdots & y_2\beta_2 & \cdots \\ \cdot & \cdot & \cdot & & \cdot & \\ \cdot & \cdot & \cdot & & \cdot & \\ \cdot & \cdot & \cdot & & \cdot & \end{vmatrix} \tag{8}$$

in which α and β are the spin wave functions specifying the spin component in a given direction z. Now in D we may add to any column a constant multiple of any other column without changing the value of the determinant. Thus we may add to the $x_i\alpha_i$ column $-X$ times the α_i column and the former column becomes $\xi_i\alpha_i$ by (5). Similarly the $y_i\beta_i$ column can be replaced by $\eta_i\beta_i$ and so on without changing the value of the determinant. It follows therefore that

$$D(\mathbf{r}_i)=D(\boldsymbol{\varrho}_i) \tag{9}$$

and from (7) $\Psi(\mathbf{r}_i)=e^{-\alpha N R^2}\Psi(\boldsymbol{\varrho}_i)$. (9′)

It should be noted that in the derivation of (9) it is essential that the $1s$ shell be complete.[3] It is also true that the separation effected in (9′) depends on the properties of the oscillator wave functions in an essential way and this result will be valid only for such wave functions.

The extension of this result to the case of higher shells is obvious. The relations (9) and (9′) will be valid in this case if only, for each kind of particle, all the shells of lower energy quantum number[2] be filled.[4] It is sufficient in each case to consider only a single monomial in the polynomial P_k since the determinant with P_k can be written as a sum of determinants in which P_k is replaced by the various monomials. In the transformation of a column containing $x^a y^b z^c$ one gets $\xi^a\eta^b\zeta^c$ plus additional monomials of lower degree. These additional monomials will coincide within a constant factor (powers of X, Y and Z) with elements in one of the columns belonging to a shell of smaller k and therefore give a vanishing contribution to the determinant.

We may now proceed to the calculation of the nuclear kinetic energy. The transformation of the kinetic energy operator in absolute coordinates, $\sum_1^N \Delta_{r_i}$, gives, as is well known, the kinetic energy operator for the center of gravity, $\Delta_{\mathbf{R}}/N$, plus an operator $\Omega_{\boldsymbol{\varrho}}$ depending only on the relative coordinates. The operator $\Omega_{\boldsymbol{\varrho}}$ is not the sum of the Laplace operators $\Delta_{\boldsymbol{\varrho}_i}$ but will contain in addition cross derivatives of the form $\mathrm{div}_{\boldsymbol{\varrho}_i}\cdot\mathrm{grad}_{\boldsymbol{\varrho}_j}$ because the $\boldsymbol{\varrho}_i$ are not independent (Eq. (6)). Therefore it is not simple to calculate the kinetic energy T', exclusive of the energy of the center of gravity, with this operator and the wave function $\Psi(\boldsymbol{\varrho}_i)$. However, T' can be easily calculated as the difference between the total kinetic energy in absolute coordinates, T, and the kinetic energy of the center of gravity, T_R. T is the sum of the kinetic energies of the individual particles in the oscillator potential. For the kinetic energy of the center of gravity we have, using (3),

$$T_R=-\frac{\hbar^2}{2MN}\frac{\int d\mathbf{R}e^{-\alpha N R^2}\Delta_{\mathbf{R}}e^{-\alpha N R^2}}{\int d\mathbf{R}e^{-2\alpha N R^2}}=\tfrac{3}{4}\hbar\omega\,; \tag{10}$$

that is, just the kinetic energy of a single $1s$ particle.

For the kinetic energy T' of a nucleus with all shells (for both particles) of energy quantum number K or less filled and with q particles in the shell of quantum number $K+1$ we find

$$\begin{aligned} T_K' &= \tfrac{1}{4}\hbar\omega\{q(2K+3)-3+\sum_{k=1}^{K}2k(k+1)(2k+1)\} \\ &= \tfrac{1}{4}\hbar\omega\{q(2K+3)-3+K(K+1)^2(K+2)\} \\ &= \tfrac{1}{4}\hbar\omega\{(2K+3)N-3 \\ &\qquad -\tfrac{1}{3}K(K+1)(K+2)(K+3)\}, \end{aligned} \tag{11}$$

in which use has been made of the fact that the total number of particles of both kinds in the

[3] Of course the $1s$ shell for one kind of particle need not be complete if there are no $2p$ particles of this kind. The relation (9) is trivial in the case of only $1s$ particles.

[4] The number of filled neutron shells need not be the same as the number of filled proton shells.

shells with quantum number k is $2k(k+1)$. The case of greatest interest is that in which the $2p$ shell is partly filled and the $1s$ shell complete. In this case $K=1$ and the kinetic energy is

$$T_1'=\frac{\hbar\omega}{4}(5q+9)=\frac{\hbar\omega}{4}(5N-11). \quad (11')$$

The difference between the result for the kinetic energy obtained here and that resulting from the use of the reduced mass is

$$\Delta T_K'=T_K/N-\tfrac{3}{4}\hbar\omega, \quad (12)$$

which for $K=1$ is

$$\Delta T_1'=\hbar\omega(N-4)/2N. \quad (12')$$

This correction varies between 25 and 50 percent of the energy $\frac{3}{4}\hbar\omega$ for the nuclei of mass number between 6 and 16, and will have the effect of raising the energy levels as formerly computed by about 2 to 4 MV for these nuclei.

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Spherical Symmetry of Self-Consistent Atomic Fields

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THE method of the self-consistent field (s. c. f.) for an N electron atom is equivalent to the assumption

$$\psi=\psi_1(1)\cdots\psi_N(N) \quad (1)$$

in the variational principle. This leads (neglecting spin terms) to the equations

$$\nabla_i^2\psi_i+(\epsilon_i-2V_i)\psi_i=0 \quad (j=1,\cdots,N), \quad (2a)$$

where

$$V_i(\mathbf{r}_j)=-Z/r_j+\sum_{k=1(k\neq j)}^{N}\int|\psi_k(\mathbf{r}_k)|^2/r_{jk}\cdot d\tau_k, \quad (2b)$$

Z being the nuclear charge, and atomic units being used. On the other hand, all calculations which have actually been made so far with the s. c. f. have proceeded on the assumption that the field for each electron is spherically symmetrical. This is effected by making the additional assumption

$$\psi_j(\mathbf{r}_j)=(2\pi)^{-\frac{1}{2}}e^{im_j\phi_j}P_{m_jl_j}(\theta_j)R_j(r_j) \quad (3)$$

in the variational principle, where we denote by $P_{ml}(\theta)$ the *normalized* tesseral harmonic $P_l^{|m|}(\cos\theta)$, m_j and l_j being the magnetic and azimuthal quantum numbers of the jth electron.

The assumption (3) is, however, incompatible with Eqs. (2a), (2b) unless all the electrons are s electrons. Excluding this special case, therefore, (3) imposes a restriction on the form of the wave function which is *additional* to that implied by (1). Consequently, although the assumption of spherical symmetry is entirely reasonable from the physical point of view and simplifies considerably the numerical work, it would appear that the generalized Eqs. (2) are more accurate than those ordinarily used, and this seems to have been the generally held opinion. If this were really the case, one might solve the more general equations by approximate methods and estimate the magnitude of the corrections that would thereby result. A closer examination, however, leads to the conclusion that if the assumption (1) is made (or the generalizations considered below), the central field assumption is, in effect, a *necessary* one if the solution obtained is to fulfil certain general requirements.

Let us first of all examine the nature of the solution of Eqs. (2). There is a degree of arbitrariness about the solution, but we may safely assume that the central field approximation is a good one. Let us, then, see what type of solution results when we solve (2) by successive approxi-