Center-of-Mass Motion in Many-Particle Systems*†

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An explicit construction is found for a unitary operator which insures the free motion of the center of mass of any many-particle wave function on which it is allowed to act. The transformation is used to calculate recoil correction terms for the internal energy and external interactions of nuclei, and some numerical evaluations are given for cases of interest. The many-body harmonic-oscillator problem is exactly soluble when one uses the transformation, and one is thus enabled to give a more general discussion of the spurious states.

I. INTRODUCTION

I t is a first law of physics that in the dynamical description of any isolated system of particles the total linear momentum is a constant of the motion. Despite this knowledge, one frequently disregards this principle in the construction of approximate wave functions (an independent-particle model for example) to describe a given state. Generally, there is good reason for this neglect, since if one extracts the proper center-of-mass (c.m.) motion for a system of A particles, the A−1 sets of spatial coordinates which remain to describe the internal motions do not treat the particles in a symmetric manner. Thus, for example, it may become very difficult to satisfy the Pauli principle for such an internal wave function.

Neglect of the c.m. motion for a system of A equally massive particles will result in errors of order 1/A in calculations of binding energies, energy-level spectra, electromagnetic moments and transition rates, β-decay matrix elements, etc. These corrections may be important for very light nuclei, provided of course one can calculate these properties to at least 1/A accuracy. Furthermore, the inclusion of c.m. motion has led to some very important qualitative revisions as, for example, the N/A factor in the dipole sum rule and the T=0 forbiddenness for E1 transitions. Another more recent development is the recognition of the spurious states.

One approach to the general c.m. problem which has been developed recently consists of introducing three extra degrees of freedom into the A-body Hamiltonian so that one has 3 c.m. coordinates in addition to 3A internal coordinates. However, in this approach one must carry along a condition of constraint which

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reduces the 3A+3 coordinates to 3A independent ones. This technique is rather cumbersome and has not contributed to an understanding of such problems as the spurious states.

In the present work we construct a unitary operator which, in a certain limit, imposes the correct c.m. motion on any many-particle wave function without changing any other over-all symmetry property, such as spin and parity. In order to achieve this, the transformation projects out of any state its translationally invariant part by referring all particle coordinates to the center of mass. Such a transformation, if carried out explicitly, would evidently be very singular since it reduces the number of degrees of freedom by three and may in this sense be thought of as being equivalent to the method of superfluous coordinates referred to above. Nevertheless, by appropriate limiting procedures the transformation can be handled and gives meaningful answers with a minimum of mathematical labor.

Rules for obtaining recoil corrections appropriate for all calculations are given in Eq. (15).

II. UNITARY TRANSFORMATION

The description of an isolated many-particle system is governed by a Hamiltonian of the form

\[ H = \sum_i (p_i^2/2m_i) + V, \]

where \( p_i \) is the momentum of the \( i \)th particle of mass \( m_i \); and \( V \) is an interaction which for the present purpose may depend only on the relative particle coordinates \( \mathbf{r}_i - \mathbf{r}_j \), the relative velocities, the spins, and the isotopic spins. Since the total momentum of the system must be conserved, the eigenfunctions of \( H \) must be translationally invariant except possibly for a trivial phase factor. More formally, one says that \( \mathbf{P} = \sum_i \mathbf{p}_i \) commutes with \( H \), and one can select the eigenfunctions of \( H \) to be simultaneously eigenfunctions of \( \mathbf{P} \) (which is the generator of infinitesimal translations). Even though in practice one cannot hope to find the exact eigenfunctions of \( H \), one would frequently like to impose the translational invariance symmetry on any approximate wave functions. The common practice of using independent-particle wave functions, referred to some particular origin (vaguely thought to be the center of mass), is clearly incompatible with this
principle. In the present study we propose to find a
transformation which makes any approximate wave
function translationally invariant.
In order to obtain such a transformation, consider that we are given a many-particle function
\[ \Phi(r_1, r_2, \cdots, r_n) = \Phi(r_i), \]
which depends\(^7\) on the particle coordinates \( r_i \). Out of this function, we wish to construct a new one,
\[ \Psi(r_i) = U(r_i) \Phi(r_i), \]
where \( U \) is some operator such that \( \Psi \) has the property
\[ \Psi(r_i + \Delta) = \Psi(r_i) \]
for arbitrary displacements of all the particle coordinates by an amount \( \Delta \). In terms of \( \Phi \), Eq. (4) reads
\[ U(r_i + \Delta) \Phi(r_i + \Delta) = U(r_i) \Phi(r_i). \]
A solution of (5) which is valid for arbitrary functions \( \Phi \) is
\[ U(r_i) = e^{-i\Delta \cdot (\mathbf{R} \cdot \mathbf{P} + \mathbf{P} \cdot \mathbf{R})}, \]
where \( \mathbf{R} \) is the c.m. operator for the system, i.e.,
\[ \mathbf{R} = \sum_i m_i / M \mathbf{r}_i; \quad M = \sum_i m_i, \]
and \( \Delta \) is a constant which is eventually allowed to become infinite.\(^8\) To show that this is the desired operator, we use Eqs. (3)–(6) as given above to obtain
\[ \Psi(r_i + \Delta) = U(r_i + \Delta) \Phi(r_i + \Delta) \]
\[ = \exp \left\{ -\frac{i}{2} \Delta \cdot (\mathbf{R} \cdot \mathbf{P} + \mathbf{P} \cdot \mathbf{R}) \right\} \Phi(r_i + \Delta), \]
which, upon using an operator identity derived in Appendix A, becomes
\[ \Psi(r_i + \Delta) = e^{-i\Delta \cdot \mathbf{P}(1 - e^{-\lambda})} \Phi(r_i + \Delta). \]
Finally, using Taylor's theorem, we have
\[ \Psi(r_i + \Delta) = U(r_i) \Phi(r_i + \Delta e^{-\lambda}), \]
which clearly satisfies (4) if we take the limit \( \Delta \to \infty \).
It is thus established that a function \( \Psi \) which is constructed from an arbitrary function \( \Phi \) in accordance with Eqs. (3) and (6), is translationally invariant.

We note that the operator \( \mathbf{R} \cdot \mathbf{P} \) is a scalar, and in addition for identical particles is symmetric under any permutation of the particle coordinates. Thus, symmetries under rotation, inversion, and particle exchange which are contained in \( \Phi \) are also present in \( \Psi \). The operator \( U \), therefore, adds new symmetries to a given function without destroying any already present.

\(^7\) We suppress all spin and isotopic-spin variables since they are clearly irrelevant for our purposes.

\(^8\) It should be kept in mind that in writing \( \mathbf{R} \) and \( \mathbf{P} \) we always mean the explicit functions of the \( r_i \) and \( p_i \) and not any new variables.

In general, one expects the functions \( \Psi \) to be structurally much more complicated than the \( \Phi \) and thus one may fear that subsequent computations using the \( \Psi \) will be too heavy a price to pay for the added symmetry. However, in practice one need never compute with \( \Psi \) but can still work with \( \Phi \) which is frequently selected for simplicities in subsequent computations. To see how this comes about, let us consider the matrix element of an operator \( O \),
\[ \langle \Psi_f | O | \Psi_i \rangle, \]
which because of (3) can be written in the form
\[ \langle U \Psi_f | O U \Psi_i \rangle = \langle \Phi_f | U' \Phi_i \rangle. \]
Inspection of (11) shows that one can calculate matrix elements with translationally invariant wave functions by using the given functions and using operators transformed according to the rule,
\[ O' = U'OU = U^{-1}O U, \]
where the second equality follows from the unitarity of \( U \) according to (6).
The problem of calculating matrix elements with \( \Psi \) is thus reduced to finding the transformed operators. Since spin and isotopic spin are invariant under \( U \), the only operators we need consider are the particle coordinates and momenta. Straightforward computation using the well-known rule
\[ e^{\delta O} e^{-\delta S} = O + [S, O] + \frac{1}{2!} [S, [S, O]] + \cdots \]
yields
\[ p_i' = U^{-1} p_i U = p_i + \frac{m_i}{M} (e^\lambda - 1) \]  
(14a)
and
\[ r_i' = U^{-1} r_i U = r_i + \mathbf{R}(e^\lambda - 1). \]  
(14b)
In particular, we note from (14a) that \( \mathbf{P} \) is transformed into \( \mathbf{P} e^{\lambda} \) which vanishes in the limit \( \Lambda \to \infty \) as we would expect from (4). It should not be surprising that, as follows from (14b), \( \mathbf{R} \) gets transformed into \( \mathbf{R} e^\lambda \) which becomes infinite in the limit. Since the commutator of \( \mathbf{P} \) and \( \mathbf{R} \) is invariant under \( U \) (which is unitary), the fact that \( \mathbf{R} \to \infty \) as \( \mathbf{P} \to 0 \) is merely the statement of the uncertainty principle. The reason that this infinity is not troublesome in practice follows from the observation that in any measurement which refers only to the internal dynamics, the operators of interest can involve only the relative positions of the particles, which, as can be seen from (14b), bring in no infinities. In cases of doubt, one should always hold off the limit on \( \Lambda \) until the end of any calculation. On the basis of this discussion then, we can expect to require only the
following transformation:
\[
\begin{align*}
  r_i - r_j &\rightarrow r_i - r_j, \\
  r_i - R &\rightarrow r_i - R, \\
  p_i &\rightarrow (m_i/M)p_i \\
  p_i/m_i &\rightarrow p_i/m_i \\
  P &\rightarrow 0.
\end{align*}
\]

Matrix elements computed by using these transformed operators with arbitrary wave functions are then equal to those computed by using translationally invariant wave functions.

As an example of the use of the transformation, let us transform the Hamiltonian given by (1). On the basis of the assumptions made about \( H \), we see that \( V \) commutes with \( R \) and \( P \) and hence with \( U \), and thus only the kinetic-energy part of \( H \) gets transformed. Using (15), we find that under \( U \), the Hamiltonian transforms according to
\[
H \rightarrow H' = H - (P^2/2M).
\]

Now we note that \( P^2/2M \) is a positive-definite operator, and hence, the expectation value of the energy in the state \( \Psi \) is lower than it is with \( \Phi \); i.e., using (3) and (16), we have
\[
(\Psi, H\Psi) = (\Psi, [H - P^2/2M]\Phi) \leq (\Phi, H\Phi).
\]

Thus, in this Rayleigh-Ritz sense, \( \Psi \) is a better approximation to the correct wave function than \( \Phi \); and further only if \( \Phi \) is already translationally invariant does the equality in (17) hold. In Appendix B, a particular example\(^9\) of an energy calculation is considered, where the c.m. motion exerts a dominating influence.

It should be emphasized that the operator \( U \) is singular and frequently care must be exercised in its use. As has been pointed out above, in all cases of doubt, one should keep \( \Lambda \) finite until the end. For example, let us consider a function \( U\Phi(r) \) appearing on the right-hand side of a matrix element. Using properties of \( U \) discussed above, we have
\[
U\Phi(r) = \left[ U\Phi(r) U^{-1} \right] U 1 = e^{-1\Lambda} \Phi(r - R(1 - e^{-\Lambda})),
\]
and we cannot take the limit on \( \Lambda \) directly. The factor of \( e^{-1\Lambda} \) in (18) can be absorbed into the integration over \( R \) and is a reflection of the fact that the volume of normalization of the c.m. coordinate has been expanded by \( U \), and also that we are left with 3 less degrees of freedom in \( \Phi(r - R) \). With this renormalization understanding, we could write
\[
U\Phi(r) = \Phi(r - R).
\]

However, once we have taken the limit on \( \Lambda \), we can never undo it, since \( r_i - R \) is invariant under \( U \) for all


\( \Lambda \) and thus
\[
U^{-1}(\Lambda) U(\infty) \Phi(r) \neq \Phi(r)
\]
for any \( \Lambda \). Nevertheless, one can get useful results out of the transformation by never tampering with the wave functions but equivalently transforming all operators according to (15). In this way, no new difficulties are encountered.

**III. ELECTROMAGNETIC MOMENTS**

With the cautions of the preceding paragraphs in mind, one can apply the \( U \) transformation to the operators for the electric and magnetic multipole interactions. However, since these operators, as usually derived, involve the particle coordinates \( r_i \) referred to some fixed origin, direct application of the transformation would yield infinite results. In order to avoid this difficulty we must redefine the interaction operators by studying the interaction with the external field involving a finite momentum transfer, and allowing the nucleus as a whole to recoil.

The initial nuclear state, chosen to be at rest, is written in accordance with (3) as
\[
\Psi_i = U\Phi_i,
\]
and the final state with some linear momentum \( \mathbf{K} \) is
\[
\Psi_f = e^{i\mathbf{K} \cdot \mathbf{R}} U\Phi_f.
\]

The interaction Hamiltonian,
\[
H' = \frac{i}{\hbar} \sum_i \left[ \mathbf{e} \cdot \mathbf{j}_i(p_i) e^{ik \cdot r_i} + e^{ik \cdot r_i} \mathbf{e} \cdot \mathbf{j}_i(p_i) \right],
\]
represents the coupling of the appropriate nuclear currents\(^9\) \( \mathbf{j}_i \) with the external field \( e^{ik \cdot r_i} \) carrying a momentum \( \mathbf{K} \). The transition matrix is then
\[
(\Psi_f, H'\Psi_i) = (\Phi_f, U^{-1} e^{-i\mathbf{K} \cdot R} \sum_i e^{ik \cdot r_i} \mathbf{e} \cdot \mathbf{j}_i(p_i)) U\Phi_i,
\]
which can be written in the form
\[
(\Phi_f, U^{-1} e^{-i\mathbf{K} \cdot R} \sum_i e^{ik \cdot r_i} \mathbf{e} \cdot \mathbf{j}_i(p_i)) U\Phi_i.
\]

Now we carry out the transformations \( U^{-1} \) \( U \) (for finite \( \Lambda \)) on each part of this operator to obtain
\[
\left( \Phi_f, \exp[\{i(K - \mathbf{K}) \cdot R\mathbf{e} \}^A] \sum_i e^{ik \cdot r_i} \mathbf{e} \cdot \mathbf{j}_i(p_i)ight)
\times \left[ \mathbf{e} \cdot \mathbf{j}_i \left( p_i + M \frac{m_i}{M} (1 - e^{-\Lambda}) \right) \right] \Phi_i.
\]
The limit \( \Lambda \to \infty \) may now be taken and, except for the factor \( \exp \{i(\mathbf{k} - \mathbf{R}) \cdot \mathbf{r} \} \), everything is obviously well defined. It is clear that as \( \Lambda \to \infty \) this questionable factor oscillates infinitely rapidly and will make the entire matrix element zero when we integrate over any of the coordinates [we recall that \( \mathbf{R} = \sum_i (m_i/M) \mathbf{r}_i \)]. The only way to avoid this calamity is to put \( \mathbf{K} = \mathbf{k} \), which eliminates this factor for all \( \Lambda \). This is of course just the statement of momentum conservation which in usual treatments comes out in the form of a delta function, resulting from an integration over the coordinate \( \mathbf{R} \).

We do not wish to treat \( \mathbf{R} \) as an independent coordinate in order to retain \( 3\Lambda \) degrees of freedom for the function \( \Phi \); yet we have been able to obtain the desired results by careful use of the c.m. transformation.

Now the remaining factors in (22) have just their customary form except for the replacements,

\[
p_i \rightarrow p_i - (m_i/M) \mathbf{P}, \quad \mathbf{r}_i \rightarrow \mathbf{r}_i - \mathbf{R}.
\]

(23)

In the simple case of no velocity-dependent forces and low-energy processes,\(^{11}\) the usual electric and magnetic multipole operators are given just by the solid harmonics\(^{12}\)

\[
X_{lm}(\mathbf{r}) = r_i Y_{lm}(\theta_i, \phi_i),
\]

and the orbital angular momentum

\[
\frac{1}{m} \mathbf{r}_i \times \mathbf{p}_i.
\]

We now include the recoil corrections by using \( X_{lm}(\mathbf{r} - \mathbf{R}) \) and \( [\mathbf{r}_i - \mathbf{R}] \times (\mathbf{p}_i - (m_i/M) \mathbf{P}) \) instead. Let us now set \( m_i/M = 1/A \), and consider a few examples. The electric dipole \((E1)\) operator becomes

\[
\sum_i e_i [\mathbf{r}_i - \mathbf{R}] = \sum_i \mathbf{r}_i [e_i - (Ze/A)]
\]

(24)

which is already familiar in the literature.\(^{13}\) The magnetic dipole \((M1)\) operator becomes (aside from spin-dependent parts which are unaffected by recoil)

\[
\sum_i \frac{e_i}{2mc} (\mathbf{r}_i - \mathbf{R}) \times (\mathbf{p}_i - \mathbf{P}) = \sum_i \mathbf{r}_i \times \mathbf{p}_i \left( e_i - \frac{2e_i}{A}\right) \frac{Ze}{A^2} + \frac{1}{2mc} \sum_{ij} \frac{\mathbf{r}_i \times \mathbf{p}_j + \mathbf{r}_j \times \mathbf{p}_i}{2mc} \left( e_i - e_j \right) \frac{Ze}{A^2}.
\]

(25)

The electric quadrupole \((E2)\) operator has exactly the same form as the \(M1\) operator except that \(\mathbf{r}_i \times \mathbf{p}_i\) is replaced by the electric quadrupole tensor \(\mathbf{r}_i \times \mathbf{r}_j - \langle \mathbf{r}_i \mathbf{r}_j \rangle \). The modifications of the \(M1\) and \(E2\) matrix elements due to recoil effects are of two kinds; first, a sort of reduced-charge correction to the usual term; and second, exchange matrix elements involving two particles in orbits differing by one unit of \(l\). For matrix elements between states each having no more than one incomplete shell (shell here means any groups of orbits having the same parity, as for example, in the harmonic oscillator), the recoil corrections can be summarized by giving to each particle in an \(l\)-orbit an effective orbital \(g\)-factor \(g_i\) with the usual magnetic-moment operator, and an effective charge \(e_q\) with the usual quadrupole operator. A straightforward calculation using (25) yields \([\text{in units of } 1/(2mc)]\)

\[
M1 = \sum_i g_i r_i \times p_i;
\]

\[
g_i = e_i + \left( -\frac{2e_i}{A} + \frac{Ze}{A^2} \right) \left[ 1 - \sum \frac{1}{(2l+1)!} \left( \frac{l}{r} \right)^l \right] \times \left[ (l + 1) (l + 2) \left( \frac{1}{|r|} \right)^l + (l - 1) \left( \frac{d}{dr} \right)^l \right] \left( \frac{d}{dr} \right)^l \left( \frac{d}{dr} \right)^l,
\]

(26)

where the matrix elements are integrals over radial functions only and the sum extends over all filled shells for which \(l' = l \pm 1\). If the states \(l, l'\) are given as the eigenfunctions of a common static potential with eigenvalues \(E_l\) and \(E_{l'}\), the term in square brackets can be more conveniently written in the form

\[
1 - \sum \frac{2m}{\hbar^2} \frac{(l - 1) (l + 2)}{2l + 1} \left( E_l - E_{l'} \right) \left( \frac{l}{r} \right)^l \left( \frac{l}{r} \right)^l.
\]

(27)

Within a shell one may have \(E2\) matrix elements which change \(l\) by 0 or \(\pm 2\). For these two cases we get two effective quadrupole charges.

\[
E2 = \sum_i e_q r_i^2 Y_{20}(\theta_i),
\]

\[
\langle l | e_q r_i^2 | l \rangle = \langle l | r^2 | l \rangle + \left( -\frac{2e_i}{A} + \frac{Ze}{A^2} \right) \left[ \langle l | r^2 | l \rangle \right] - \frac{(2l - 1) (2l + 3)}{2l + 1} \sum \left( \frac{l}{r} \right)^l \left( \frac{l}{r} \right)^l,
\]

(28)

\[
\langle l \pm 2 | e_q r_i^2 | l \rangle = \langle l \pm 2 | r^2 | l \rangle + \left( -\frac{2e_i}{A} + \frac{Ze}{A^2} \right) \left[ \langle l \pm 2 | r^2 | l \rangle \right] - 2 \sum \left( \frac{l \pm 2}{r} \right)^l \left( \frac{l \pm 2}{r} \right)^l,
\]

(29)

where again all matrix elements mean integrals over radial functions only and the states \(l'\) which contribute
in any matrix elements $\langle l' | r | l \rangle$ are the closed shells for which $l' - l = \pm 1$. It should be repeated that these formulas for the recoil-corrected $g_i$ and $e_q$ are correct only for matrix elements involving states in which the orbits of all $l$-shells which have at least one but less than $2 \times 2 \times (2l + 1)$ particles have a common parity.

The recoil corrections for $M1$ and $E2$ matrix elements involving ground or low states in the harmonic-oscillator shell model may be readily evaluated, using Eqs. (27), (28), and (29); and one gets exactly zero in all cases as a result of a cancellation between the direct and exchange terms. This result is at first sight surprising and somewhat disappointing too, since one might have hoped to explain by this effect at least part of the small magnetic-moment deviation from the Schmidt value for $N^{16}$ and $O^{17}$. Now, however, the vanishing of recoil corrections to all multipole moments can be seen as a general property of the harmonic-oscillator model within the limitations specified in reference 12. The result follows from the fact, first noted by Bethe and Rosen, that the antisymmetrized wave function for the lowest states in the harmonic-oscillator shell model are automatically translationally invariant except for a factor $\exp[-(Av/2)R^2]$. Thus, if one carried out a coordinate transformation which separated internal coordinates from the c.m. coordinates, one would have a wave function which contained only $s$-state components in the coordinate $R$. All the recoil-correction terms we have derived for the multipole operators involve $R$ and $P$ in some vector, or higher rank tensor form; thus, these correction terms all average to zero under integration over $R$.\(^{16}\)

For a shell model with other than harmonic-oscillator radial wave functions the recoil corrections to $M1$, $E2$, etc., moments will not vanish, but for any reasonably shaped central potential they are expected to remain quite small. These terms have been evaluated for the infinite square-well wave functions with the following results: a particle in the first $p$-shell has

$$g_i = e_i + \left( -\frac{2e_i}{A} \right) \frac{Ze}{A^2} [0.032] \tag{30a}$$

$$\langle l | e_q | l \rangle = e_i + \left( -\frac{2e_i}{A} \right) \frac{Ze}{A^2} [-0.25] \tag{30b}$$

and for a particle in the first $d$-shell, the numbers in square brackets in Eqs. (30) are replaced by 0.029 and $-0.19$, respectively.

The magnetic moments of the double magic nuclei $A^{16}$ and $O^{17}$ both depart from the Schmidt values by about 0.02 magnetic magneton, but the recoil corrections as calculated with these numbers is only one-tenth of this (although in the right direction). It is conceivable that with wave functions given by a "wine-bottle-shaped" central potential, as could be given in a Hartree-Fock calculation by exchange forces, these corrections might increase to a significant fraction of the 0.02-nm discrepancy; but at this time they are too small to consider. For the Li isotopes the quadrupole recoil correction is, using the numbers given above, only about 5%, and thus negligible. Similarly, only about $-6\%$ of the small quadrupole moment of the odd-neutron nucleus $O^{17}$ is given by the preceding calculation.\(^{14}\)

The sole exception to the rule that recoil corrections vanish in the harmonic-oscillator model, and are thus very small in similar models, is the electric monopole operator,

$$\sum_i r_i' \left[ e_i - \frac{Ze}{A} \right] + \sum_{ij} r_i r_j' \left[ \frac{Ze}{A^2} \right], \tag{31}$$

in which the recoil terms are scalar in $R$. This operator enters into the description of elastic electron scattering at not too high energies and also governs zero-zero transitions. The inversion of the nuclear mean-square radius given by electron scattering according to the shell model will involve recoil corrections of magnitude $1/A$. The recoil terms may be of some importance in an analysis of the monopole transition in $O^{18}$ (it allows a "two-particle jump"), but we have carried out no such calculation. For the monopole transition in $C^{12}$ the recoil terms, just as the usual operator,\(^{17}\) give zero matrix element as long as one allows no particles to move out of the $1p$-shell.

The scattering of high-energy $\gamma$ rays on electrons is governed, in the Born approximation, by operators of the form $e^{ik \cdot r' \cdot r}$. For calculations with a shell model or any other nontranslationally invariant approximate wave function, this operator is replaced by $e^{ik \cdot (r' - r)}$ which in general involves the coordinates of all $A$ particles at once. A few such terms have been calculated for some simple nuclei and the results yield simple $1/A$ corrections which are of interest in further studies.\(^{18}\)

In conclusion, we may state that we have studied the recoil corrections to operators describing various interactions of the nucleus with external fields, but that within the framework of the existing shell-model theory, we have found no numerically important corrections.

IV. SPURIOUS STATES

Elliott and Skyrme\(^3\) first noted the existence of spurious states for Fermi-Dirac particles coupled together in pairs by harmonic-oscillator potentials and


\(^{15}\) See reference 3 and also J. P. Elliott and T. H. R. Skyrme, Nuovo cimento 4, 164 (1956).

\(^{16}\) One knows anyway from the strong $E2$ transition of the 872-kev level of $O^{17}$ that some collective excitations (or configuration mixing) is important here.

\(^{17}\) B. F. Sherman and D. G. Ravenhall, Phys. Rev. 103, 949 (1956).

\(^{18}\) S. D. Drell and C. Schwartz (to be published).
gave a prescription for removing them. They showed that some states did not correspond to excitation of the internal coordinates but represented merely motion of the center of mass. This particular case of harmonic oscillator potentials will be discussed further in the next section. The existence of spurious states is not confined to the harmonic oscillator for which the analysis is reasonably simple, but may arise, for example, whenever one uses any sort of independent-particle description and thus some care may be required in interpretations of results. As has been pointed out, one may deduce qualitatively as well as quantitatively incorrect results by neglecting c.m. motion.

The basic problem of the spurious states lies in the fact that for purposes of describing internal dynamics one would like to use eigenfunctions of $H$, Eq. (1), which involve $3A$ coordinates (for reasons of simplicity in including antisymmetrization, etc.), while in actuality one should really use solutions involving $3A-3$ degrees of freedom. Now, following the customary procedure one writes down a set of functions $\Phi_n$ which are approximate eigenfunctions of (1) belonging to the eigenvalue $E_n$ and which are constructed without regard for c.m. motions. However, using our prescription one would take the functions $\Psi_n = U\Phi_n$ to be the eigenfunctions of $H$ with eigenvalues $E_n$; that is, we have

$$H\Psi_n = E_n\Psi_n, \quad (32)$$

which implies directly the equation,

$$(H - P^2/2M)\Phi_n = E_n\Phi_n, \quad (33)$$

It follows that the functions $\Phi_n$ are really eigenfunctions of $H - P^2/2M$ rather than of $H$. Also, using (4), we see that (32) can be rewritten in the form

$$(H - P^2/2M)\Psi_n = E_n\Psi_n, \quad (34)$$

which is formally the same equation as (33). Now $\Psi_n$ involves only $3A-3$ degrees of freedom since it is independent of $\mathbf{R}$, while $\Phi_n$ which formally satisfies the same equation, has its full $3A$ degrees of freedom. Hence, it seems reasonable to conclude that there may exist more states $\Phi_n$ than $\Psi_n$. We conclude thus that the operator $U$ has the potentiality of taking several states $\Phi_n^{(o)}$ into a single state $\Psi_n$. Following Elliott and Skyrme, of the several states $\Phi_n^{(o)}$ one would keep one, call the remainder spurious and ignore them, in constructing a complete set of internal states. That is, one must first recognize that several $\Phi_n^{(o)}$ correspond to the same $\Psi_n$ and then count all of these $\Phi_n^{(o)}$ only once. Further, since $U$ is unitary, a collection of $\Phi_n^{(o)}$ which belong to the same $\Psi_n$ must have the same energy.

Thus, we see that it is vital for the description of the internal dynamics of a system of particles to confine oneself to translationally invariant functions. Otherwise, spurious states enter and one might, for example, assign incorrect weights to levels or possibly (as first pointed out by Elliott and Skyrme) predict energy levels where none might exist. In calculating matrix elements, one can completely rely on the operator $U$ to remove spurious states without taking the trouble to recognize them explicitly.

V. HARMONIC OSCILLATOR

The quantum-mechanical problem of many particles bound by Hooke’s law forces between all pairs can be solved exactly by going to the normal modes. However, it is in general difficult to pick the individual particle coordinate out of the normal coordinates in order to apply antisymmetrization according to the Pauli principle. Use of the transformation for the c.m. motion yields a very convenient solution to this problem.

The Hamiltonian for this system of $A$ particles is

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} (r_i - r_j)^2, \quad (35)$$

where we have set all masses and spring constants equal for the situation of interest. We describe the translationally invariant solution $\Psi$ of $H$ via our unitary c.m. transformation, $\Psi = U\Phi$, and $\Phi$ satisfies $H'\Phi = E\Phi$, where

$$H' = H - (P^2/2Am).$$

It is now convenient to break up $H'$ into two parts:

$$H' = H_o + H_1,$$

$$H_o = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \frac{kA}{2},$$

$$H_1 = \frac{1}{A} \sum_{i=1}^{A} \sum_{j=1}^{A} \left[ \frac{p_i \cdot p_j}{m} + \frac{A k}{2} (r_i - r_j) \cdot (r_i - r_j) \right], \quad (36)$$

The exact solution of this transformed harmonic oscillator problem can be found once one notices the important fact that $H_1$ commutes with $H_o$. For then, the functions which diagonalize the matrix of $H_o$ also diagonalize the total $H'$, and the eigenfunctions of $H_o$ are exactly the shell-model wave functions describing $A$ particles moving in a common oscillator potential. We have thus proved that the exact solution $\Psi$ for the many-body oscillator problem is just the shell-model wave function $\Phi$, corrected for center-of-mass motion.

Special attention must be given to the case of degenerate states $\Phi$, for then one will have to diagonalize the (finite) matrix of $H_1$; in all nondegenerate states one need only take the expectation value of $H_1$ as an energy shift. The effect of $H_1$ on certain groups of degenerate solutions will lead to the identification of spurious states, and this problem will now be studied in detail.

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19 It is interesting to note that one could add a two-body spin-orbit force, $(\sigma_1 + \sigma_2) \cdot [(r_i - r_j) \times (p_i - p_j)]$ to (35) and still have the exact solution in shell-model form since this interaction also commutes with $H_o + H_1$. 

---
First note that \( H_1 \) can be written

\[
H_1 = -\frac{(P^2/2\hbar^2) - (A^2\hbar^2/2R^2)}{A} \tag{37}
\]

and if one took the (improper) liberty of speaking of \( R \) as a new coordinate, independent of the \( r_i \), one would say that the c.m. moved in an h-o potential with the same frequency \( \omega = (A\hbar/m)^{1/2} \) as each individual particle.\(^{14}\) The diagonalization of \( H_1 \) would then correspond to separating the eigenstates of the c.m. motion. If any group of states differs only in the state of the c.m. motion, only one—say the 1s state—need be retained to describe the internal energy state of the system; the others would be called spurious states which have appeared because of the excessive degrees of freedom employed. This freehand description may be of use in discussing the rigorous analysis to follow.

Let us rewrite \( H_1 \) once again:

\[
H_1 = -\frac{\hbar^2}{2A} \sum_i \{a_i\, a_i' + a_i'\, a_i \} \tag{38}
\]

where \( a_i = (2\hbar\omega)^{-1/2}(p_i - im\omega) \) and \( a_i' \), its Hermitian conjugate, are the familiar lowering and raising operators. The first term in this expression for \( H_1 \) is handled in the obvious way. Matrix elements of the second term, which we shall call \( \alpha \), have the following selection rules: \( \alpha \) is diagonal in the total orbital angular momentum and all spins; only two individual particles may change their states, with one jumping up one oscillator quantum and the other jumping down by one shell, each changing its orbital quantum number \( l \) by \pm 1 unit.

For states in which there is only one shell incompletely filled and any number of other filled shells, \( (H_1) \) is diagonal in the orbital classification of states \( \Phi \) of \( H_0 \) and there are no spurious states. This results from the fact that \( \alpha \) will have only exchange matrix elements involving particles in the other closed shells. Because of the spherical symmetry of the closed shells the matrix of \( \alpha \) is effectively a scalar quantity in the coordinates of the particles in the unfilled shells and cannot mix any states. For such cases the energy shift due to the diagonal matrix elements of \( H_1 \) works out to be \( H_1 = -\frac{\hbar^2}{2} \omega \). One is drawn to interpret this as a subtraction of the energy of the c.m. moving in a 1s orbit.\(^{14}\) When there are two or more unfilled shells, there may be exchange matrix elements of \( \alpha \) between particles in these two shells which can mix up the orbital occupations. We shall look at the excited states of closed-shell nuclei as examples.

Consider a nucleus whose ground state has all shells closed and the last closed shell has total quantum number \( N_f \); this state, which we shall call \( \Phi_0 \), has \( L = S = T = 0 \) and its energy is shifted \(-\frac{3}{2}\hbar\omega \) by \( (H_0, H_{1}\Phi_0) \). The individual particle orbits are described by the total quantum number \( N_a \) where the energy of the orbit is given by \( E_a = (N_a + \frac{1}{2})\hbar\omega \) and the orbital angular-momentum quantum numbers allowed within any shell are \( l = N, N - 2, N - 4, \ldots \). The first excited states, \( \Phi_1 \), arise from moving one particle out of the \( N \) shell and putting it into the \( N + 1 \) shell. There are several orbits \( l_1, l_1', \ldots \) in the shell \( N \) from which to take this particle and several orbits \( l_2, l_2' \) · · · in the shell \( N + 1 \) into which to put it. Each \( \Phi_1 \) will thus be labeled by the orbital quantum numbers \( l_1, l_2 \) describing the hole and particle orbits, respectively, and the total quantum numbers \( L, S, T \) as well as \( M \) values for the latter. We have of course

\[
(\Phi_1 | (l_1 l_2 T S L)H_0 | (l_1' l_2' T' S' L')) = \delta_{l_1 l_1'} \delta_{l_2 l_2'} \delta_{T T'} \delta_{S S'} \delta_{L L'} \tag{39}
\]

and the matrix of \( H_1 \) in the states \( \Phi_0 \) is also diagonal in the quantum numbers \( T S L \), but \( H_1 \) is not in general diagonal in \( l_1, l_2 \). We then calculate by standard techniques

\[
(l_1 l_2 T S L)H_1 (l_1' l_2' T' S' L') = \delta_{l_1 l_1'} \delta_{l_2 l_2'} \left(-\frac{3 + N + 1}{2A}\right)\hbar\omega.
\]

The double-barred matrices are the reduced-matrix elements as defined by Racah,\(^{20}\) and the only non-vanishing reduced-matrix elements of \( a, a' \) are the following:

\[
\langle N + 1, l + 1 | a'| N, l \rangle = \langle l + 1 | (N + l + 3)^{\delta_{l-l_1}} \tag{41a}
\]

\[
\langle N + 1, l - 1 | a'| N, l \rangle = \langle l(N - l - 2)^{\delta_{l-l_1}} \tag{41b}
\]

and

\[
\langle N', l' | a'| N, l \rangle = (-1)^l N(N-l)^{\delta_{l-l_1}} \tag{42a}
\]

\[
\langle N, l | a'| N', l' \rangle = (-1)^l N(N-l)^{\delta_{l-l_1}} \tag{42b}
\]

It is seen from (40) that only in the states for which \( T = S = 0, L = 1 \) (i.e., \( 1^p \) states) can \( H_1 \) mix orbits. For all other states, \( H_1 \) is diagonal and we have

\[
\langle H_1 \rangle = -\frac{3 + N + 1}{2A}\hbar\omega = -\frac{3}{2A}\hbar\omega.
\]

which is the same shift suffered by the ground state \( \Phi_0 \). The matrix of \( H_1 \) in the \( 1^p \) states will have a diagonal element of \(-\frac{3}{2A}\hbar\omega \) and also the contribution from the second term in (40) which we now evaluate for the general case.

First note that this matrix can be written in product

form

\[ \langle l_1 l_2 | H_1 + \frac{p^2}{2m} | l_1' l_2' \rangle = \frac{4\hbar \omega}{3A} \langle l_1 | a | l_2 \rangle \langle a | l_1' \rangle \]

and for any matrix \( A_{a b} \) which can be written \( A_{a b} = A_a B_b \), one can find the eigenvalues directly. There exists a unitary matrix \( T \) which can diagonalize \( A_{a b} \):

\[ \sum_{a , \gamma} T_{a \gamma} a^* A_{a \gamma} T_{b \gamma} = \delta_a \delta_{ab} ; \]

but since \( A_{a b} \) factors, we have

\[ (\sum_{a} A_{a} T_{a a}^*) (\sum_{a} B_{a} T_{a a}^*) = \delta_a \delta_{ab} , \quad (44) \]

and since the two factors on the left are independent, we must have \( \sum_{a} A_{a} T_{a a}^* = 0 \) except for one particular value of \( a \), which we call \( a_0 \); or \( \sum_{a} B_{a} T_{a a}^* = 0 \) except for one particular value of \( \delta \), which we call \( \delta_0 \). In either case the eigenvalues of \( a_0 \) of \( A_{a b} \) are thus all zero except for one of them, \( a_0 \), which may be nonzero and is just equal to the trace of \( A_{a b} \). For our problem, the desired trace is

\[ \frac{4\hbar \omega}{3A} \sum \left[ (l_1 + 1)(N + l_1 + 3) + l_1 (N - l_1 + 2) \right] , \]

which works out to be exactly \(-\hbar \omega\). It also follows that the relative probabilities of the orbital components of this one state are proportional to the corresponding diagonal matrix elements.

Thus, we see that out of the many degenerate excited states at energy \( \hbar \omega \) above the singly degenerate \( ^{11}S \) ground state, one particular state of character \( ^{11}P \) has been separated out and moved down to exactly the energy level of the ground state. This special \( ^{11}P \) state, which will be recognized as a spurious state, has the orbital composition

\[ \Phi_{a b} = \sum_{l_1, l_2} \Phi(Nl_1^{-1}, N + 1 l_2^{11}P) \left( \frac{1}{3A} (l_1 + l_2 + 1) \right)^3 \times \left[ 2N + 4 + l_2(l_2 + 1) - l_1(l_1 + 1) \right] . \quad (45) \]

Following Elliott and Skyrme, it will then be found that one can write \( \Phi_{a b} = RU \Phi_0 \) (within a constant). When we now apply the \( U \) operator to get the physical states, we have \( \Psi_0 = U \Phi_0 \) for the ground state; and for the aforementioned spurious state we obtain \( U \Phi_0 = UU^{-1} \Phi_0 = \lim (A \rightarrow \infty) e^{-\lambda A} RU \Phi_0 \), which becomes a null state. The more general statement is that whenever some model states \( \Phi_0 \) can be written in terms of another (apparently independent) model state \( \Phi_0 \) as \( \Phi_0 = F_0(R) \Phi_0 \), then, when the \( U \) operator is applied, we have

\[ \Psi_0 = U \Phi_0 \]

\[ \Psi_0 = U F_0(R) \Phi_0 = F_0(0) U \Phi_0 . \quad (46) \]

Thus, the states \( \Psi_0, \psi \) are not linearly independent and correspond to only a single eigenstate; one can then work with only one of the states, say \( \Psi_0 \), and the other \( \Psi_1 \) are called spurious. We have remarked before that since \( U \) is a unitary operator, the states \( \Phi_1 \) which are spurious with respect to some \( \Phi_0 \) must have exactly the same energy as \( \Phi_0 \) in the model.

For higher excited states one expects to find several spurious states. Among the second excited states of a closed shell there should be two spurious states—\( ^{11}S \) and \( ^{11}D \)—corresponding to the physical ground state with \( 2\hbar \omega \) of excitation in the c.m. coordinate \( R \). There would also be a number of spurious states found by adding one \( \hbar \omega \) of c.m. excitation (i.e., a \( p \)-state) to each of the proper states at one \( \hbar \omega \) excitation.

The detailed working out of all these results is simple only for the harmonic oscillator, and it is fortunate that this model does appear to be a good starting point for the description of light nuclei. For any other shell model the spurious states do exist although one will not be able to display them so neatly. However, as long as one uses the formalism of the \( U \) transformation and works only with translationally invariant operators, no errors will be made. Thus, for example, if one sets out to diagonalize an energy matrix in some representation not free of spurious states, the labor might be increased by the superfluous degree of freedom, but consistent use of the \( U \) operator would prevent the spurious components from coupling with the proper ones under any measurement referring to the internal dynamics.

VI. ACKNOWLEDGMENTS

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APPENDIX A

In order to prove the identity, Eq. (8) = Eq. (9), we shall prove the following operator identity. If \( A, B \) are arbitrary operators which obey

\[ [A, B] = \alpha B , \]

where \( \alpha \) is a constant \( c \) number, then

\[ e^{A + B} = e^A \exp \left( B - \frac{1 - e^{-\alpha}}{\alpha} \right) . \quad (A2) \]

To prove this we write

\[ e^{(A + B)} = e^{A} B e^{B \lambda} \]

where \( \lambda \) is a parameter which we eventually set equal to 1 and \( O(\lambda) \) is a \( c \)-number function of \( \lambda \), and \( O(0) = 0 \). We differentiate (A3) with respect to \( \lambda \), and on suitable rearrangement we obtain

\[ \frac{dO}{d\lambda} = e^{-B \lambda} e^{A} B \lambda A \lambda B \lambda , \]

which upon application of (13) and (A1) reduces to

\[ \frac{dO}{d\lambda} = e^{-\lambda A} . \]
This equation has as its solution (subject to the above boundary conditions) \( O(\lambda) = (1/\alpha)(1-e^{-\lambda \alpha}) \), and substituting this into (A3) and setting \( \lambda = 1 \) we obtain the desired result (A2).

The identity Eq. (8) = Eq. (9) now follows if we take

\[
A = -\frac{i}{\hbar} \mathbf{R} \cdot \mathbf{P} + \mathbf{P} \cdot \mathbf{R} \quad \text{and} \quad B = -i \mathbf{A} \cdot \mathbf{P},
\]

in which case \( \alpha = \lambda \).

In passing we may also point out that, if one uses techniques similar to those above, the unitary transformation \( e^{-i \mathbf{P} \cdot \mathbf{R}} \) induces a linear transformation among the coordinates and momenta. Straightforward calculation shows that

\[
e^{-i \mathbf{P} \cdot \mathbf{R}} e^{-i \mathbf{P} \cdot \mathbf{R}} = \sum_i r_i (e^{i \mathbf{P} \cdot \mathbf{R}})_{ii},
\]

where \( (e^{i \mathbf{P} \cdot \mathbf{R}})_{ii} = 1 + \alpha r_i (1/2) \sum_k a_{ik} a_{ki} + \cdots \).

Using this, we can induce some linear transformations among coordinates and momenta of wave functions and operators. It is not clear that all linear transformations can easily be written in this form, but on occasion it may be useful to have the foregoing formal techniques available.

**APPENDIX B**

Since the usual Hartree-Fock approximation (antisymmetrized-product wave function) is not translationally invariant, one can improve this wave function by using the c.m. operator \( U \). Instead of the original Hamiltonian \( H \), one now seeks Hartree-Fock solutions for the transformed Hamiltonian

\[
U^{-1}HU = H - \mathbf{P}^2/2M,
\]

which would generally appear (for a system of \( A \) equally massive particles) as

\[
\left( \frac{A-1}{A} \right) \sum_i \frac{\mathbf{p}_i^2}{2m} - \sum_{i \neq j} \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{2Am} + V.
\]

Aviles and Jastrow\textsuperscript{21} have recently reported results of a Hartree-Fock calculation (ignoring the c.m. motion) for He\textsuperscript{4}. With a two-body force

\[
V(r) = V_o P_\alpha e^{-\alpha r}/\mu r,
\]

where \( \mu^3 = 1.17 \times 10^{-13} \) cm, \( V_o = -67.3 \) Mev, and \( P_\alpha \) (as averaged in He\textsuperscript{4}) = 0.845, they find a binding energy of only 10 Mev. This result is very much less than the binding energy of 55 Mev obtained by Irving\textsuperscript{22} for the same problem by the use of the trial function

\[
\Phi = \left| \sum_i r_i^3 \right|^2 \exp \left| -\alpha \left[ \sum_{i < j} r_{ij}^2 \right] \right|.
\]

Since for He\textsuperscript{4} one has all particles in an \( s \)-state, the terms \( \mathbf{p}_i \cdot \mathbf{p}_j \) \((i \neq j)\) do not contribute; and so the c.m. corrected Hamiltonian differs from the original one only by a factor \( 3/4 \) in the kinetic-energy term.

Using, as an approximation to the Hartree-Fock solution, the trial 1s orbital \( \Phi = e^{-\alpha r}(1 + \alpha r) \) with this simply modified Hamiltonian, we have obtained a binding energy of 44 Mev at \( \mu/\alpha = 0.33 \). The complete Hartree-Fock solution should come even closer to Irving’s result.

The recoil correction for He\textsuperscript{4}—taking the Hartree-Fock result from 18\% to 80\% of Irving’s answer—is so very large because the kinetic and potential energies are both very large (200 Mev) in this particular problem. Thus, a 25\% decrease in the kinetic energy gives a much larger percent-wise increase in the difference between kinetic and potential energies.


\textsuperscript{22} J. Irving, Phil. Mag. 42, 338 (1951).